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*inventor
search*

FILE COVERS 1907 - 17 Mar 2003 VOL 138 ISS 12

FILE LAST UPDATED: 16 Mar 2003 (20030316/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

L1 1131 SEA FILE=CAPLUS ABB=ON CUNNINGHAM J?/AU
L2 921 SEA FILE=CAPLUS ABB=ON GORDON G?/AU
L3 54 SEA FILE=CAPLUS ABB=ON NICKOLS G?/AU
L4 38 SEA FILE=CAPLUS ABB=ON RUMINSKI P?/AU
L5 20 SEA FILE=CAPLUS ABB=ON WESTLIN W?/AU
L6 579 SEA FILE=CAPLUS ABB=ON ROGERS T?/AU
L7 2 SEA FILE=CAPLUS ABB=ON L1 AND L2 AND L3 AND L4 AND L5 AND L6)

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L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:290790 CAPLUS

DOCUMENT NUMBER: 136:310191

TITLE: Preparation of peptidyl integrin antagonists for use in combination with a chemotherapeutic agent for treatment of neoplasia

INVENTOR(S): Cunningham, Jay; Gordon, Gary B.;
Nickols, G. Allen; Westlin, William F.
; Rogers, Thomas Edward; Ruminski, Peter Gerrard

#6

PATENT ASSIGNEE(S): USA

SOURCE: U.S., 35 pp., Cont.-in-part of U.S. Ser. No. 34,270, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

INT. PATENT CLASSIF.:

MAIN: A61K031-70

SECONDARY: A61K031-66; A61K031-505; A61K031-335; A61K031-24

US PATENT CLASSIF.: 514034000

CLASSIFICATION: 34-3 (Amino Acids, Peptides, and Proteins)

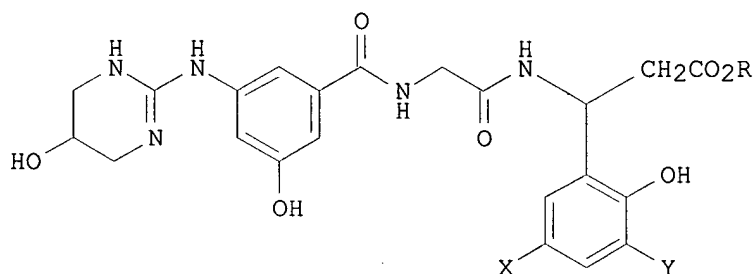
Section cross-reference(s): 1

FAMILY ACC. NUM. COUNT: 5

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 6372719 B1 20020416 US 1999-262725 19990304
ZA 9904406 A 20000211 ZA 1999-4406 19990211
WO 2000051686 A1 20000908 WO 2000-US3705 20000301
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
EP 1161280 A1 20011212 EP 2000-914580 20000301
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO
JP 2002538177 T2 20021112 JP 2000-602347 20000301
US 2003050250 A1 20030313 US 2001-16146 20011210
PRIORITY APPLN. INFO.: US 1998-34270 B2 19980304
US 1999-262725 A 19990304
WO 2000-US3705 W 20000301
OTHER SOURCE(S): MARPAT 136:310191
GRAPHIC IMAGE:



ABSTRACT:

Peptides I (R = H, alkyl; X, Y = halo) were prepd. as .alpha.v.beta.3 integrin antagonists which in combination with a chemotherapeutic agent (cisplatin, cyclophosphamide, 5-fluorouracil, doxorubicin and taxol) are used for treatment of neoplasia. Thus, 3-bromo-5-chloro-2-hydroxy-.beta.-[[2-[[[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxypyrimidin-2-yl)amino]phenyl]carbonyl]amino]acetyl]amino]benzenepropanoic acid trifluoroacetate was prepd. by peptide coupling of N-glycyl-.beta.-(3-bromo-5-chloro-2-hydroxyphenyl)-.beta.-aminopropionic acid Et ester with 3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxypyrimidin-2-yl)amino]benzoic acid. Peptides I delayed the growth of tumors in mice, particularly when combined with a chemotherapeutic agent.

SUPPL. TERM: beta3 integrin antagonist chemotherapeutic agent; peptide
integrin antagonist prepn antitumor
INDEX TERM: Amino acids, preparation
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(esters, .beta.-; prepn. of peptidyl integrin antagonists
for use in combination with a chemotherapeutic agent for
treatment of neoplasia)
INDEX TERM: Neoplasm
(metastasis; prepn. of peptidyl integrin antagonists for
use in combination with a chemotherapeutic agent for
treatment of neoplasia)
INDEX TERM: Angiogenesis inhibitors
Antitumor agents

Human

(prepn. of peptidyl integrin antagonists for use in combination with a chemotherapeutic agent for treatment of neoplasia)

INDEX TERM:

Peptides, preparation

ROLE: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptidyl integrin antagonists for use in combination with a chemotherapeutic agent for treatment of neoplasia)

INDEX TERM:

Integrins

ROLE: BSU (Biological study, unclassified); BIOL (Biological study)

(.alpha.v.beta.3; prepn. of peptidyl integrin antagonists for use in combination with a chemotherapeutic agent for treatment of neoplasia)

INDEX TERM:

7440-70-2, Calcium, biological studies

ROLE: BSU (Biological study, unclassified); BIOL (Biological study)

(hypercalcemia; prepn. of peptidyl integrin antagonists for use in combination with a chemotherapeutic agent for treatment of neoplasia)

INDEX TERM:

243135-63-9P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)- 243135-65-1P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)- 243135-66-2P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-iodo-2-hydroxyphenyl)- 243135-67-3P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)- 243135-68-4P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-chloro-3-iodo-2-hydroxyphenyl)- 243135-69-5P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dibromo-2-hydroxyphenyl)- 243135-70-8P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)-, (3S)- 243135-71-9P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, monohydrochloride, (3S)- 243135-72-0P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3S)- 243135-74-2P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-chloro-5-iodo-2-hydroxyphenyl)- 243135-75-3P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-iodo-2-hydroxyphenyl)- 243135-76-4P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-diiodo-2-hydroxyphenyl)- 243135-78-6P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dibromo-2-hydroxyphenyl)-, (3S)- 243135-79-7P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-

pyrimidinyl)amino]benzoyl]glycyl-3-(5-chloro-3-iodo-2-hydroxyphenyl)-, (3S)- 243135-80-0P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-2-hydroxy-3-iodophenyl)-, (3S)- 243135-81-1P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-diiodo-2-hydroxyphenyl)-, (3S)- 290826-47-0P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, compd. with trifluoromethanol
ROLE: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptidyl integrin antagonists for use in combination with a chemotherapeutic agent for treatment of neoplasia)

INDEX TERM: 50-18-0, Cyclophosphamide 51-21-8, 5-Fluorouracil
15663-27-1, Cisplatin 23214-92-8, Doxorubicin
33069-62-4, Taxol

ROLE: PAC (Pharmacological activity); THU (Therapeutic use);
BIOL (Biological study); USES (Uses)

(prepn. of peptidyl integrin antagonists for use in combination with a chemotherapeutic agent for treatment of neoplasia)

INDEX TERM: 75-15-0, Carbon disulfide, reactions 90-59-5,
3,5-Dibromosalicylaldehyde 90-60-8, 3,5-Dichlorosalicylaldehyde 108-24-7, Acetic anhydride
616-29-5, 1,3-Diamino-2-hydroxypropane 635-93-8,
5-Chlorosalicylaldehyde 1761-61-1, 5-Bromosalicylaldehyde
3970-21-6, Ethane, 1-(chloromethoxy)-2-methoxy- 5292-43-3,
tert-Butyl bromoacetate 19652-32-5, 3-Bromo-5-chlorosalicylaldehyde 20989-17-7, s Phenylglycinol
76045-71-1, 3-Amino-5-hydroxybenzoic acid 290826-72-1,
Glycine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]-

ROLE: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of peptidyl integrin antagonists for use in combination with a chemotherapeutic agent for treatment of neoplasia)

INDEX TERM: 19652-33-6P, Benzaldehyde, 5-bromo-3-chloro-2-hydroxy-
20300-61-2P, 2H-1-Benzopyran-2-one, 6,8-dichloro-
21524-15-2P, 2H-1-Benzopyran-2-one, 6,8-dibromo-
51656-70-3P, Zinc, bromo[2-(1,1-dimethylethoxy)-2-oxoethyl]-
55107-70-5P, 2(1H)-Pyrimidinethione, tetrahydro-5-hydroxy-
188813-14-1P, Benzenepropanoic acid, .beta.-amino-3,5-dichloro-2-hydroxy-, ethyl ester, hydrochloride
188813-16-3P, 2H-1-Benzopyran-2-one, 8-bromo-6-chloro-
188813-17-4P, 2H-1-Benzopyran-2-one, 4-amino-8-bromo-6-chloro-3,4-dihydro-, hydrochloride 215124-03-1P,
Benzaldehyde, 5-chloro-2-hydroxy-3-iodo- 240424-42-4P,
Benzaldehyde, 3,5-dichloro-2-[(2-methoxyethoxy)methoxy]-
240424-47-9P, Benzenepropanoic acid, .beta.-amino-3,5-dichloro-2-hydroxy-, ethyl ester, (.beta.S)-,
4-methylbenzenesulfonate (salt) 240424-52-6P,
Benzenepropanoic acid, .beta.-amino-3-bromo-5-chloro-2-hydroxy-, ethyl ester, (.beta.S)- 240424-53-7P,
Benzenepropanoic acid, .beta.-amino-3-bromo-5-chloro-2-hydroxy-, ethyl ester, (.beta.S)-, 4-methylbenzenesulfonate (salt) 240424-54-8P, Benzaldehyde, 5-bromo-3-chloro-2-[(2-methoxyethoxy)methoxy]- 240424-57-1P, Benzenepropanoic acid, 5-bromo-3-chloro-2-[(2-methoxyethoxy)methoxy]-.beta.-[(phenylmethylene)amino]-, 1,1-dimethylethyl ester,

(.beta.S)- 240424-59-3P, Benzenepropanoic acid, .beta.-amino-5-bromo-3-chloro-2-hydroxy-, ethyl ester, (.beta.S)-, 4-methylbenzenesulfonate (salt) 240424-63-9P, Benzaldehyde, 3,5-diiodo-2-[(2-methoxyethoxy)methoxy]- 240424-64-0P, Benzenepropanoic acid, .beta.-[[(1S)-2-hydroxy-1-phenylethyl]amino]-3,5-diiodo-2-[(2-methoxyethoxy)methoxy]-, 1,1-dimethylethyl ester, (.beta.S)- 240424-66-2P, Benzenepropanoic acid, .beta.-amino-2-hydroxy-3,5-diiodo-, (.beta.S)-, 4-methylbenzenesulfonate (salt) 243135-83-3P, .beta.-Alanine, N-[(1,1-dimethylethoxy)carbonyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, ethyl ester 243135-84-4P, .beta.-Alanine, glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, ethyl ester, monohydrochloride 243135-85-5P, Benzenepropanoic acid, .beta.-amino-3-bromo-5-chloro-2-hydroxy-, ethyl ester, hydrochloride 243135-86-6P, .beta.-Alanine, N-[(1,1-dimethylethoxy)carbonyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, ethyl ester 243135-87-7P, .beta.-Alanine, glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, ethyl ester, monohydrochloride 243135-89-9P, 2H-1-Benzopyran-2-one, 4-amino-6,8-dibromo-3,4-dihydro-, hydrochloride 243135-90-2P, Benzenepropanoic acid, .beta.-amino-3,5-dibromo-2-hydroxy-, ethyl ester, hydrochloride 243135-91-3P, .beta.-Alanine, N-[(1,1-dimethylethoxy)carbonyl]glycyl-3-(3,5-dibromo-2-hydroxyphenyl)-, ethyl ester 243135-92-4P, .beta.-Alanine, glycyl-3-(3,5-dibromo-2-hydroxyphenyl)-, ethyl ester, monohydrochloride 243135-93-5P, 2H-1-Benzopyran-2-one, 6-bromo-8-chloro- 243135-94-6P, Benzenepropanoic acid, .beta.-amino-5-bromo-3-chloro-2-hydroxy-, ethyl ester, hydrochloride 243135-95-7P, 2H-1-Benzopyran-2-one, 6-chloro-8-iodo- 243135-97-9P, 2H-1-Benzopyran-2-one, 4-amino-6-chloro-3,4-dihydro-8-iodo-, hydrochloride 243135-98-0P, Benzenepropanoic acid, .beta.-amino-5-chloro-2-hydroxy-3-iodo-, ethyl ester, hydrochloride 243135-99-1P, .beta.-Alanine, N-[(1,1-dimethylethoxy)carbonyl]glycyl-3-(5-chloro-3-iodo-2-hydroxyphenyl)-, ethyl ester 243136-00-7P, .beta.-Alanine, glycyl-3-(5-chloro-3-iodo-2-hydroxyphenyl)-, ethyl ester, monohydrochloride 243136-01-8P, Benzaldehyde, 5-bromo-2-hydroxy-3-iodo- 243136-04-1P, Benzoic acid, 3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]-, monohydrochloride 243136-05-2P, .beta.-Alanine, N-[(1,1-dimethylethoxy)carbonyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, ethyl ester, (3S)- 243136-06-3P, .beta.-Alanine, glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, ethyl ester, monohydrochloride, (3S)- 243136-07-4P, Benzenepropanoic acid, 3-bromo-5-chloro-2-hydroxy-.beta.-[[(phenylmethoxy)carbonyl]amino]-, ethyl ester, (.beta.S)- 243136-08-5P, .beta.-Alanine, N-[(1,1-dimethylethoxy)carbonyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, ethyl ester, (3S)- 243136-09-6P, .beta.-Alanine, glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, ethyl ester, monohydrochloride, (3S)- 243136-10-9P, Benzaldehyde, 5-chloro-3-iodo-2-[(2-methoxyethoxy)methoxy]- 243136-13-2P, .beta.-Alanine, glycyl-3-(5-chloro-3-iodo-2-hydroxyphenyl)-, ethyl ester, monohydrochloride, (3S)- 243136-15-4P, Benzaldehyde, 3,5-dibromo-2-[(2-methoxyethoxy)methoxy]- 243136-16-5P, Benzenepropanoic acid, 3,5-dibromo-.beta.-[[(1S)-2-hydroxy-1-phenylethyl]amino]-2-[(2-methoxyethoxy)methoxy]-, 1,1-dimethylethyl ester, (.beta.S)- 243136-20-1P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, ethyl ester, (3S)- 243136-25-6P,

.beta.-Alanine, glycyl-3-(3,5-diiodo-2-hydroxyphenyl)-, monohydrochloride, (3S)- 243136-27-8P, Benzenepropanoic acid, .beta.-amino-5-chloro-2-hydroxy-3-iodo-, ethyl ester, (.beta.S)-, 4-methylbenzenesulfonate (salt) 243136-28-9P, .beta.-Alanine, glycyl-3-(5-bromo-3-iodo-2-hydroxyphenyl)-, ethyl ester, monohydrochloride 243136-29-0P, .beta.-Alanine, glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)-, ethyl ester, monohydrochloride, (3S)- 247100-86-3P, .beta.-Alanine, glycyl-3-(3,5-dibromo-2-hydroxyphenyl)-, ethyl ester, monohydrochloride, (3S)- 247101-34-4P, .beta.-Alanine, glycyl-3-(5-bromo-2-hydroxy-3-iodophenyl)-, ethyl ester, monohydrochloride 287485-08-9P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, ethyl ester, (3S)- 290826-49-2P, 5-Pyrimidinol, hexahydro-2-(methylthio)-, monohydriodide 290826-50-5P, 1(2H)-Pyrimidinecarboxylic acid, tetrahydro-5-hydroxy-2-(methylthio)-, 1,1-dimethylethyl ester 290826-51-6P, 3-Pentanone, 1-[3,5-dichloro-2-[(2-methoxyethoxy)methoxy]phenyl]-1-[[[(1R)-2-hydroxy-1-phenylethyl]amino]-4,4-dimethyl- 290826-52-7P, Benzeneethanol, .beta.-[[[3-bromo-5-chloro-2-[(2-methoxyethoxy)methoxy]phenyl]methylene]amino]-, (.beta.R)- 290826-53-8P, Benzenepropanoic acid, 3-bromo-5-chloro-.beta.-[[[(1R)-2-hydroxy-1-phenylethyl]amino]-2-[(2-methoxyethoxy)methoxy]-, 1,1-dimethylethyl ester 290826-54-9P, Benzenepropanoic acid, 3-bromo-5-chloro-2-hydroxy-.beta.-[(phenylmethoxy)carbonyl]amino]-, ethyl ester 290826-55-0P, Benzeneethanol, .beta.-[[[5-bromo-3-chloro-2-[(2-methoxyethoxy)methoxy]phenyl]methylene]amino]-, (.beta.R)- 290826-56-1P, Benzenepropanoic acid, 5-bromo-3-chloro-.beta.-[[[(1R)-2-hydroxy-1-phenylethyl]amino]-2-[(2-methoxyethoxy)methoxy]-, 1,1-dimethylethyl ester 290826-58-3P, Benzenepropanoic acid, 5-chloro-.beta.-[[[(1R)-2-hydroxy-1-phenylethyl]amino]-3-iodo-2-[(2-methoxyethoxy)methoxy]-, 1,1-dimethylethyl ester 290826-59-4P, .beta.-Alanine, N-[(1,1-dimethylethoxy)carbonyl]glycyl-3-(5-chloro-3-iodo-2-hydroxyphenyl)-, ethyl ester, (3S)-, mono(4-methylbenzenesulfonate) (salt) 290826-61-8P, Benzenepropanoic acid, .beta.-amino-3,5-dibromo-2-hydroxy-, 1,1-dimethylethyl ester, (.beta.S)-, 4-methylbenzenesulfonate (salt) 290826-67-4P, .beta.-Alanine, glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)-, ethyl ester, monohydrochloride 290826-70-9P, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3S)-, mono(trifluoroacetate) (salt) 290826-71-0P, .beta.-Alanine, N-[(1,1-dimethylethoxy)carbonyl]glycyl-3-(2-hydroxy-3,5-diiodophenyl)-, (3S)-

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of peptidyl integrin antagonists for use in combination with a chemotherapeutic agent for treatment of neoplasia)

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD.

REFERENCE(S): (1) Anon; WO 9708145 1997 CAPLUS
(2) Anon; WO 9814192 1998 CAPLUS
(3) Anon; WO 9831359 1998 CAPLUS
(4) Carter; Chemotherapy of Cancer, sec ed 1981, P107
(5) Fields, G; Exp Opin Ther Patents 1998, V8(6), P633

CAPLUS

- (6) Hong, H; J Med Chem 1997, V40, P930 CAPLUS
(7) Nicklaus, M; J Med Chem, 7th ed 1997, V40, P920 CAPLUS
(8) Pommier, Y; Antiviral Chemistry & Chemotherapy 1997,
V8(6), P463 CAPLUS
(9) Rogers; US 6013651 A 2000 CAPLUS

L7 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:628046 CAPLUS

DOCUMENT NUMBER: 133:223050

TITLE: Preparation of peptidyl integrin antagonists for use
in combination with a chemotherapeutic agent for
treatment of neoplasiaINVENTOR(S): Cunningham, Jay; Gordon, Gary B.;
Nickols, G. Allen; Westlin, William F.
; Rogers, Thomas E.; Ruminski, Peter
G. #6

PATENT ASSIGNEE(S): G.D. Searle & Co., USA

SOURCE: PCT Int. Appl., 120 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

INT. PATENT CLASSIF.:

MAIN:

SECONDARY:

A61P035-00

A61K031-505; A61K033-24; A61K031-675; A61K031-704;
A61K031-335; A61K031-505; A61K031-24; A61K031-675;
A61K031-505; A61K031-505; A61K031-505; A61K031-704;
A61K031-505; A61K031-505; A61K031-335

CLASSIFICATION: 34-3 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 1

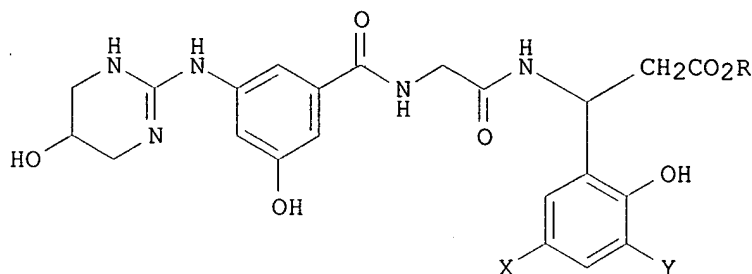
FAMILY ACC. NUM. COUNT: 5

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000051686	A1	20000908	WO 2000-US3705	20000301
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 6372719	B1	20020416	US 1999-262725	19990304
EP 1161280	A1	20011212	EP 2000-914580	20000301
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
JP 2002538177	T2	20021112	JP 2000-602347	20000301
PRIORITY APPLN. INFO.:			US 1999-262725	A 19990304
			US 1998-34270	B2 19980304
			WO 2000-US3705	W 20000301
OTHER SOURCE(S):	MARPAT 133:223050			
GRAPHIC IMAGE:				

C22H23BrClN5O7

Stereo: ns



ABSTRACT:

Peptides I (R = H, alkyl; X, Y = halo) were prepd. as .alpha.v.beta.3 integrin antagonists which in combination with a chemotherapeutic agent (cisplatin, cyclophosphamide, 5-fluorouracil, doxorubicin and taxol) are used for treatment of neoplasia. Thus, 3-bromo-5-chloro-2-hydroxy-.beta.-[[2-[[[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxypyrimidin-2-yl)amino]phenyl]carbonyl]amino]acetyl]amino]benzenepropanoic acid trifluoroacetate was prepd. by peptide coupling of N-glycyl-.beta.-(3-bromo-5-chloro-2-hydroxyphenyl)-.beta.-aminopropionic acid Et ester with 3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxypyrimidin-2-yl)amino]benzoic acid. Peptides I delayed the growth of tumors in mice, particularly when combined with a chemotherapeutic agent.

SUPPL. TERM: peptide integrin antagonist prepn antitumor
INDEX TERM: Amino acids, preparation
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(esters, .beta.-; prepn. of peptidyl integrin antagonists for use in combination with a chemotherapeutic agent for treatment of neoplasia)
INDEX TERM: Neoplasm
(metastasis; prepn. of peptidyl integrin antagonists for use in combination with a chemotherapeutic agent for treatment of neoplasia)
INDEX TERM: Angiogenesis
Antitumor agents
(prepn. of peptidyl integrin antagonists for use in combination with a chemotherapeutic agent for treatment of neoplasia)
INDEX TERM: Peptides, preparation
ROLE: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of peptidyl integrin antagonists for use in combination with a chemotherapeutic agent for treatment of neoplasia)
INDEX TERM: Integrins
ROLE: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(.alpha.v.beta.3; prepn. of peptidyl integrin antagonists for use in combination with a chemotherapeutic agent for treatment of neoplasia)
INDEX TERM: 7440-70-2, Calcium, biological studies
ROLE: BSU (Biological study, unclassified); BIOL (Biological study)
(hypercalcemia; prepn. of peptidyl integrin antagonists

for use in combination with a chemotherapeutic agent for treatment of neoplasia)

INDEX TERM:

50-18-0P, Cyclophosphamide 51-21-8P, 5-Fluorouracil
15663-27-1P, Cisplatin 23214-92-8P, Doxorubicin
33069-62-4P, Taxol 243135-63-9P 243135-65-1P
243135-66-2P 243135-67-3P 243135-68-4P 243135-69-5P
243135-70-8P 243135-71-9P 243135-72-0P 243135-74-2P
243135-75-3P 243135-76-4P 243135-78-6P 243135-79-7P
243135-80-0P 243135-81-1P 290826-47-0P
ROLE: BAC (Biological activity or effector, except adverse);
BSU (Biological study, unclassified); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological
study); PREP (Preparation); USES (Uses)

(prepn. of peptidyl integrin antagonists for use in
combination with a chemotherapeutic agent for treatment
of neoplasia)

INDEX TERM:

75-15-0, Carbon disulfide, reactions 90-59-5,
3,5-Dibromosalicylaldehyde 90-60-8, 3,5-
Dichlorosalicylaldehyde 108-24-7, Acetic anhydride
616-29-5, 1,3-Diamino-2-hydroxypropane 635-93-8,
5-Chlorosalicylaldehyde 1761-61-1, 5-Bromosalicylaldehyde
3970-21-6 5292-43-3, tert-Butyl bromoacetate 19652-32-5,
3-Bromo-5-chlorosalicylaldehyde 20989-17-7, s
Phenylglycinol 76045-71-1, 3-Amino-5-hydroxybenzoic acid
290826-72-1

ROLE: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of peptidyl integrin antagonists for use in
combination with a chemotherapeutic agent for treatment
of neoplasia)

INDEX TERM:

19652-33-6P 20300-61-2P 21524-15-2P 51656-70-3P
55107-70-5P 188813-14-1P 188813-16-3P 188813-17-4P
215124-03-1P 240424-42-4P 240424-47-9P 240424-52-6P
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243135-98-0P 243135-99-1P 243136-00-7P 243136-01-8P
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290826-61-8P 290826-67-4P 290826-70-9P 290826-71-0P

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)

(prepn. of peptidyl integrin antagonists for use in
combination with a chemotherapeutic agent for treatment
of neoplasia)

REFERENCE COUNT:

3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD.

REFERENCE(S):

- (1) Cousins, R; WO 9814192 A 1998 CAPLUS
- (2) Desai, B; WO 9708145 A 1997 CAPLUS
- (3) Duggan, M; WO 9831359 A 1998 CAPLUS

=> d his 18

(FILE 'CAPLUS' ENTERED AT 16:51:50 ON 17 MAR 2003)

FILE 'REGISTRY' ENTERED AT 16:54:11 ON 17 MAR 2003

FILE 'CAPLUS' ENTERED AT 16:54:22 ON 17 MAR 2003

{SEL RN }

FILE 'REGISTRY' ENTERED AT 16:54:30 ON 17 MAR 2003

L8 { 104 S E1-E104 }

FILE 'CAPLUS' ENTERED AT 16:55:33 ON 17 MAR 2003

=> fil reg; d scan l8

FILE 'REGISTRY' ENTERED AT 16:56:06 ON 17 MAR 2003

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STRUCTURE FILE UPDATES: 16 MAR 2003 HIGHEST RN 499182-00-2

DICTIONARY FILE UPDATES: 16 MAR 2003 HIGHEST RN 499182-00-2

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

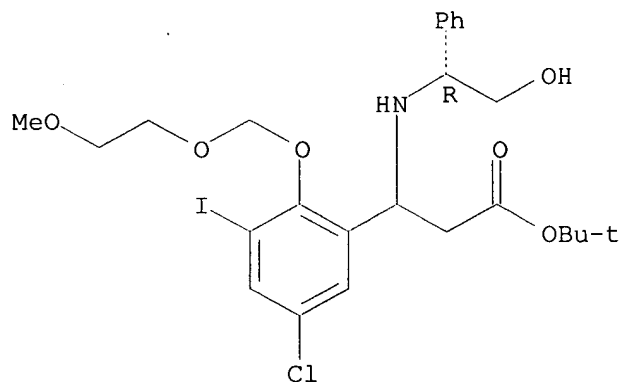
*Reg. 1314
records
from
inventors'
work*

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Benzenepropanoic acid, 5-chloro-.beta.-[[(1R)-2-hydroxy-1-phenylethyl]amino]-3-iodo-2-[(2-methoxyethoxy)methoxy]-, 1,1-dimethylethyl ester (9CI)

MF C25 H33 Cl I N O6

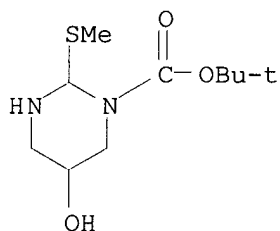
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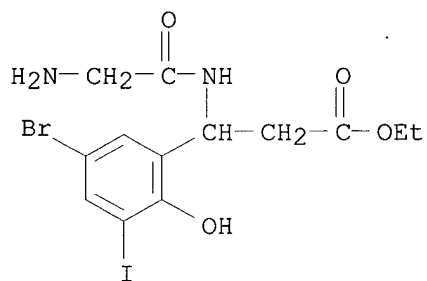
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):104

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 1(2H)-Pyrimidinecarboxylic acid, tetrahydro-5-hydroxy-2-(methylthio)-,
1,1-dimethylethyl ester (9CI)
MF C10 H20 N2 O3 S



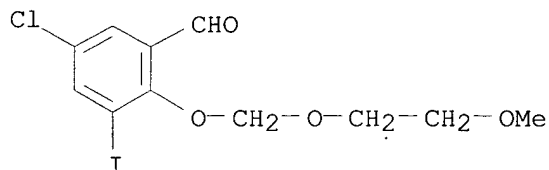
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, glycyl-3-(5-bromo-3-iodo-2-hydroxyphenyl)-, ethyl ester,
monohydrochloride (9CI)
MF C13 H16 Br I N2 O4 . Cl H



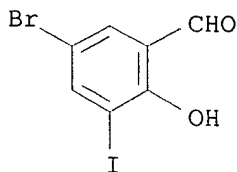
● HCl

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzaldehyde, 5-chloro-3-iodo-2-[(2-methoxyethoxy)methoxy]- (9CI)
MF C11 H12 Cl I O4



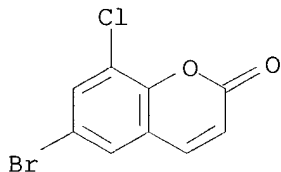
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzaldehyde, 5-bromo-2-hydroxy-3-iodo- (9CI)
MF C7 H4 Br I O2



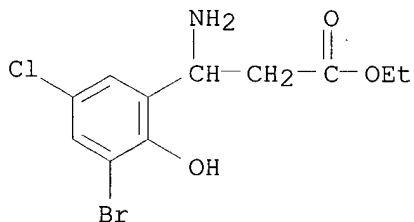
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2H-1-Benzopyran-2-one, 6-bromo-8-chloro- (9CI)
MF C9 H4 Br Cl O2



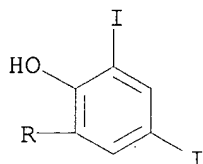
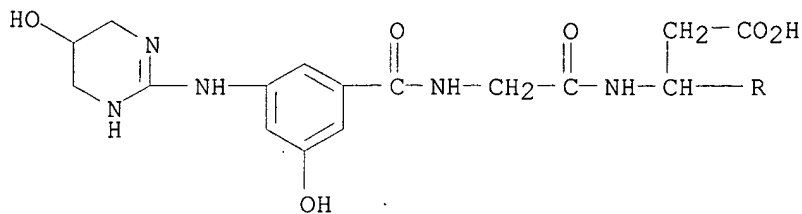
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzenepropanoic acid, .beta.-amino-3-bromo-5-chloro-2-hydroxy-, ethyl
ester, hydrochloride (9CI)
MF C11 H13 Br Cl N O3 . Cl H



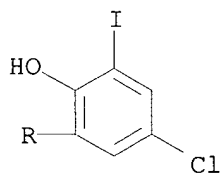
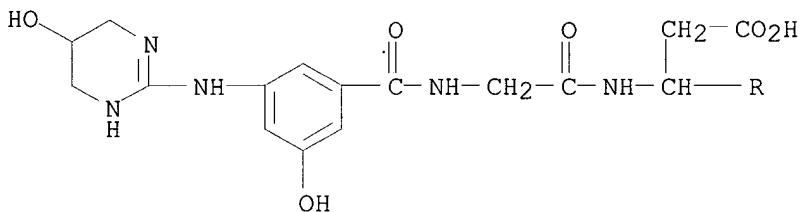
● HCl

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-
pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-diiodo-2-hydroxyphenyl)- (9CI)
MF C22 H23 I2 N5 O7



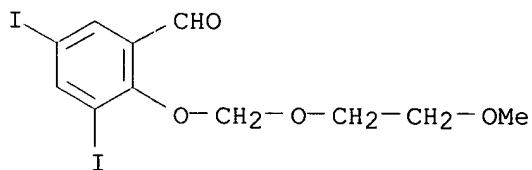
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-chloro-3-iodo-2-hydroxyphenyl)-
(9CI)
MF C22 H23 Cl I N5 O7



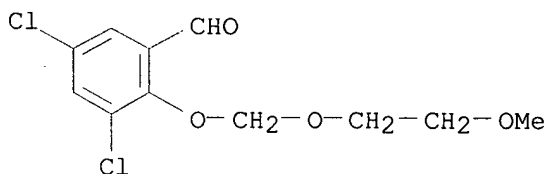
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzaldehyde, 3,5-diiodo-2-[(2-methoxyethoxy)methoxy]- (9CI)
MF C11 H12 I2 O4



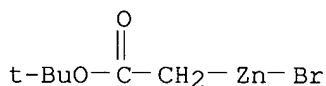
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzaldehyde, 3,5-dichloro-2-[(2-methoxyethoxy)methoxy]- (9CI)
MF C11 H12 Cl2 O4

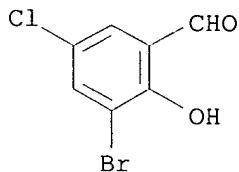


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Zinc, bromo[2-(1,1-dimethylethoxy)-2-oxoethyl]- (9CI)
MF C6 H11 Br O2 Zn
CI COM

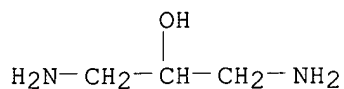


L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzaldehyde, 3-bromo-5-chloro-2-hydroxy- (9CI)
MF C7 H4 Br Cl O2



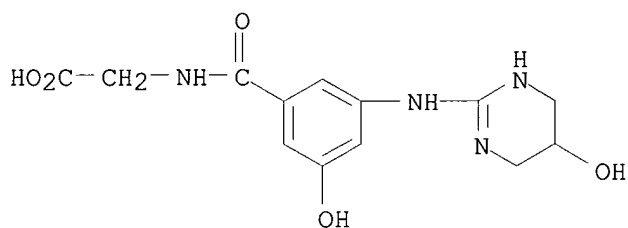
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2-Propanol, 1,3-diamino- (6CI, 7CI, 8CI, 9CI)
MF C3 H10 N2 O
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

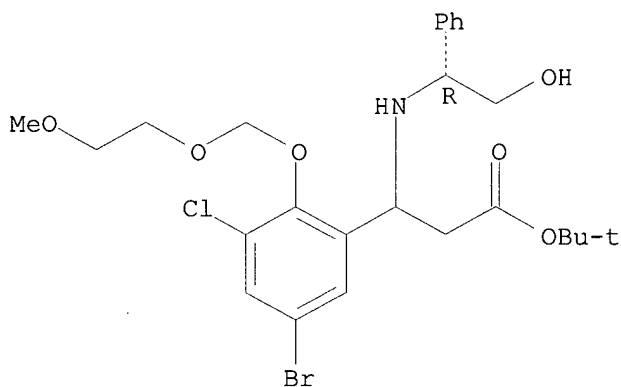
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Glycine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]- (9CI)
MF C13 H16 N4 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

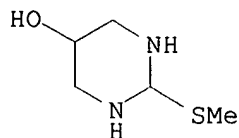
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzenepropanoic acid, 5-bromo-3-chloro-.beta.-[[(1R)-2-hydroxy-1-phenylethyl]amino]-2-[(2-methoxyethoxy)methoxy]-, 1,1-dimethylethyl ester (9CI)
MF C25 H33 Br Cl N O6

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 5-Pyrimidinol, hexahydro-2-(methylthio)-, monohydriodide (9CI)
MF C5 H12 N2 O S . H I

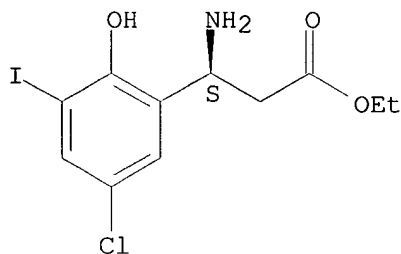


● HI

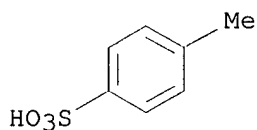
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzenepropanoic acid, .beta.-amino-5-chloro-2-hydroxy-3-iodo-, ethyl
ester, (.beta.S)-, 4-methylbenzenesulfonate (salt) (9CI)
MF C11 H13 Cl I N O3 . C7 H8 O3 S

CM 1

Absolute stereochemistry.

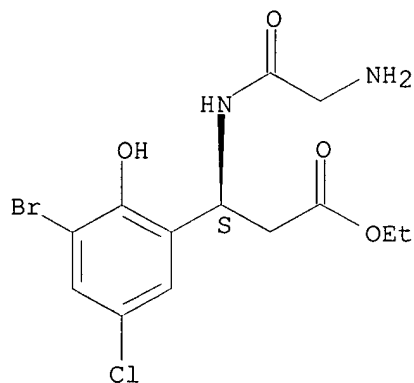


CM 2



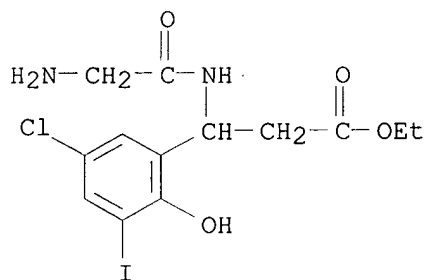
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, ethyl ester,
monohydrochloride, (3S)- (9CI)
MF C13 H16 Br Cl N2 O4 . Cl H

Absolute stereochemistry.



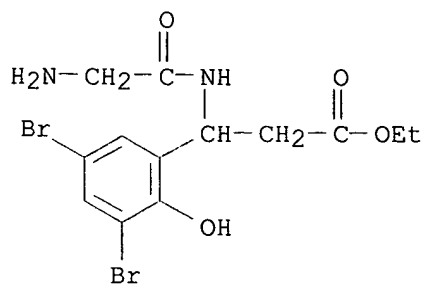
● HCl

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN .beta.-Alanine, glycyl-3-(5-chloro-3-iodo-2-hydroxyphenyl)-, ethyl ester,
 monohydrochloride (9CI)
 MF C13 H16 Cl I N2 O4 . Cl H



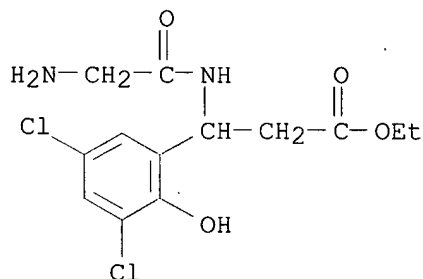
● HCl

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN .beta.-Alanine, glycyl-3-(3,5-dibromo-2-hydroxyphenyl)-, ethyl ester,
 monohydrochloride (9CI)
 MF C13 H16 Br2 N2 O4 . Cl H



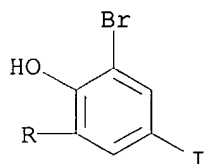
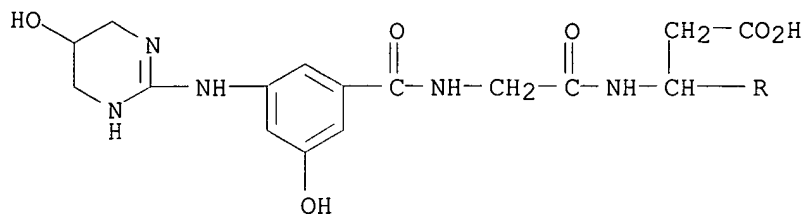
● HCl

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, glycy-3-(3,5-dichloro-2-hydroxyphenyl)-, ethyl ester,
monohydrochloride (9CI)
MF C13 H16 Cl2 N2 O4 . Cl H



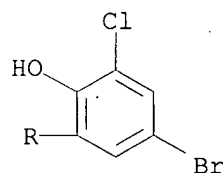
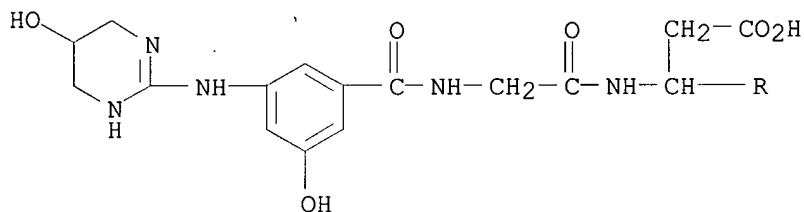
● HCl

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-
pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-iodo-2-hydroxyphenyl)- (9CI)
MF C22 H23 Br I N5 O7



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)-(9CI)
MF C22 H23 Br Cl N5 O7

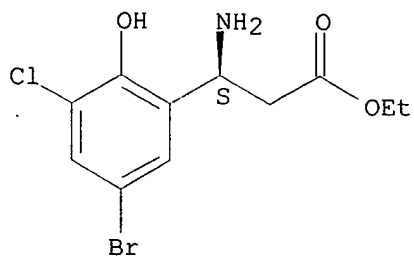


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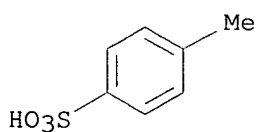
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzenepropanoic acid, .beta.-amino-5-bromo-3-chloro-2-hydroxy-, ethyl ester, (.beta.S)-, 4-methylbenzenesulfonate (salt) (9CI)
MF C11 H13 Br Cl N O3 . C7 H8 O3 S

CM 1

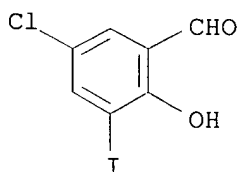
Absolute stereochemistry. Rotation (+).



CM 2



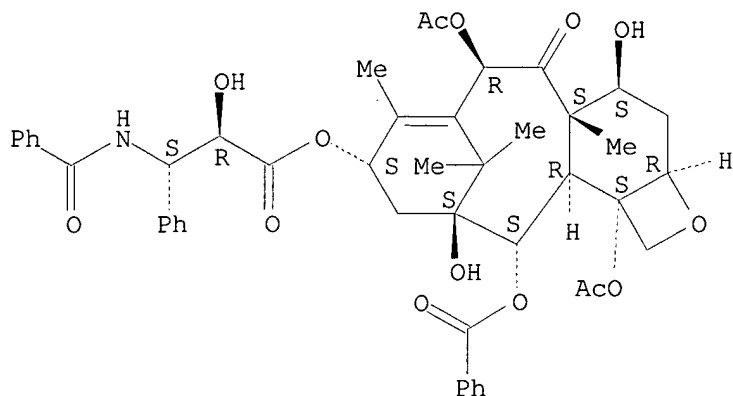
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzaldehyde, 5-chloro-2-hydroxy-3-iodo- (9CI)
 MF C7 H4 Cl I O2



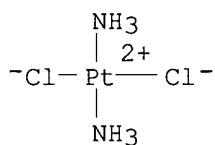
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzenepropanoic acid, .beta.-(benzoylamino)-.alpha.-hydroxy-,
 (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-
 2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-
 tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl
 ester, (.alpha.R,.beta.S)- (9CI)
 MF C47 H51 N O14
 CI COM

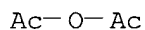
Absolute stereochemistry. Rotation (-).



L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Platinum, diamminedichloro-, (SP-4-2)- (9CI)
 MF Cl2 H6 N2 Pt
 CI CCS, COM



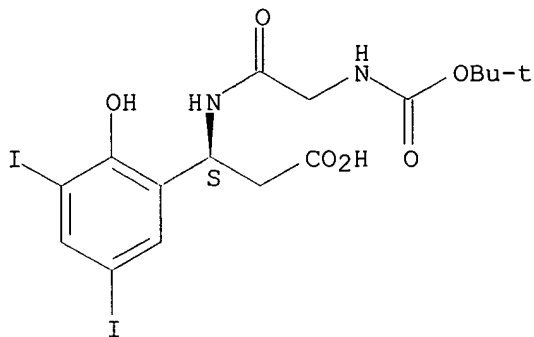
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Acetic acid, anhydride (9CI)
 MF C4 H6 O3
 CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN .beta.-Alanine, N-[(1,1-dimethylethoxy)carbonyl]glycyl-3-(2-hydroxy-3,5-diiodophenyl)-, (3S)- (9CI)
 MF C16 H20 I2 N2 O6

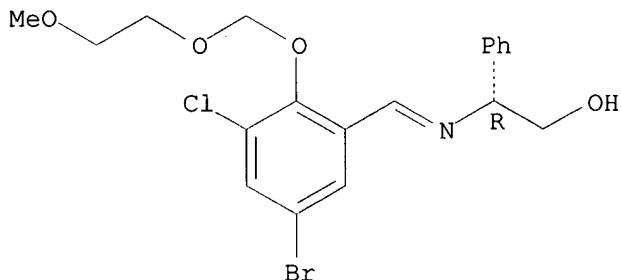
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzeneethanol, .beta.-[[[5-bromo-3-chloro-2-[(2-methoxyethoxy)methoxy]phenyl]methylene]amino]-, (.beta.R)- (9CI)
 MF C19 H21 Br Cl N O4

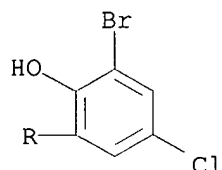
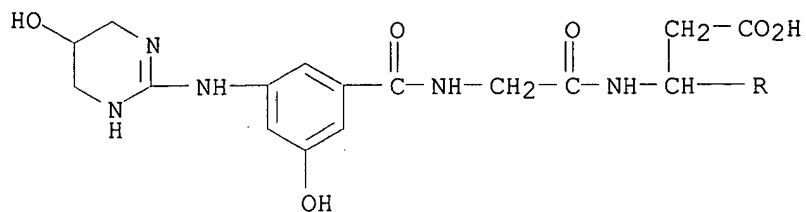
Absolute stereochemistry.
 Double bond geometry unknown.



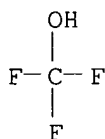
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, compd. with trifluoromethanol (9CI)
 MF C22 H23 Br Cl N5 O7 . x C H F3 O

CM 1

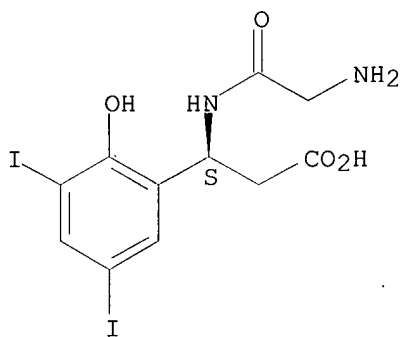


CM 2



L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN .beta.-Alanine, glycyl-3-(3,5-diiodo-2-hydroxyphenyl)-, monohydrochloride,
 (3S)- (9CI)
 MF C11 H12 I2 N2 O4 . Cl H

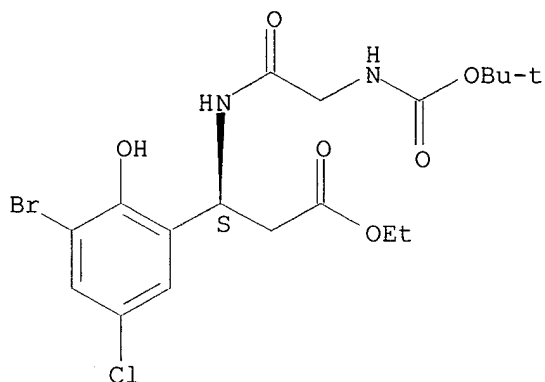
Absolute stereochemistry.



● HCl

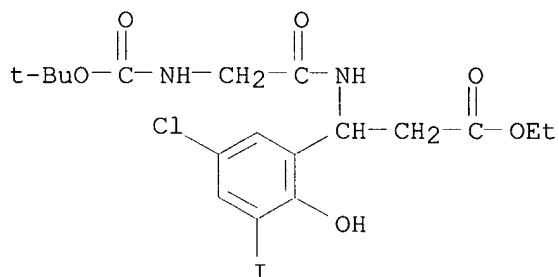
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN .beta.-Alanine, N-[(1,1-dimethylethoxy)carbonyl]glycyl-3-(3-bromo-5-chloro-
 2-hydroxyphenyl)-, ethyl ester, (3S)- (9CI)
 MF C18 H24 Br Cl N2 O6

Absolute stereochemistry.



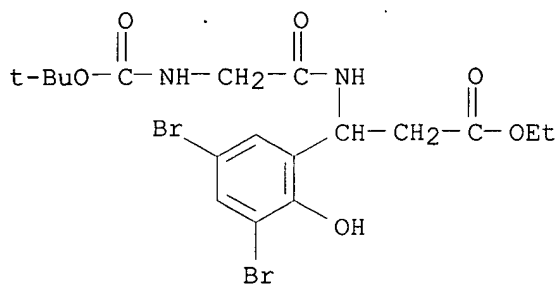
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, N-[(1,1-dimethylethoxy)carbonyl]glycyl-3-(5-chloro-3-iodo-
2-hydroxyphenyl)-, ethyl ester (9CI)
MF C18 H24 Cl I N2 O6



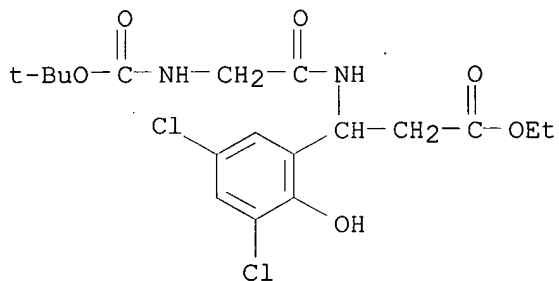
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, N-[(1,1-dimethylethoxy)carbonyl]glycyl-3-(3,5-dibromo-2-
hydroxyphenyl)-, ethyl ester (9CI)
MF C18 H24 Br2 N2 O6



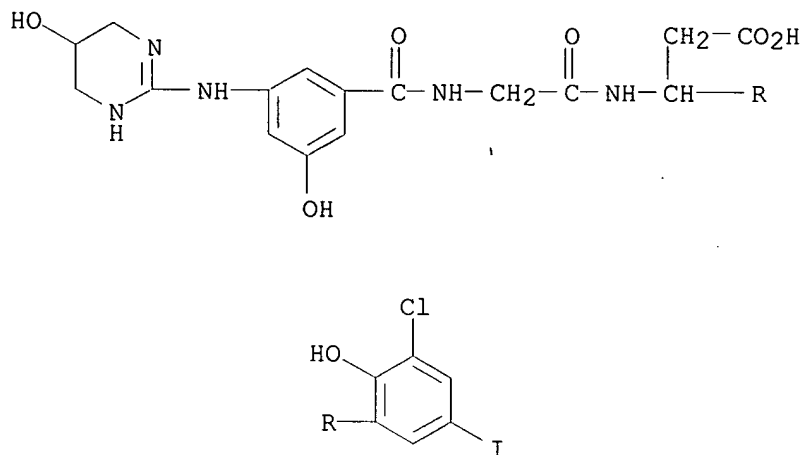
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, N-[(1,1-dimethylethoxy)carbonyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, ethyl ester (9CI)
MF C18 H24 Cl2 N2 O6



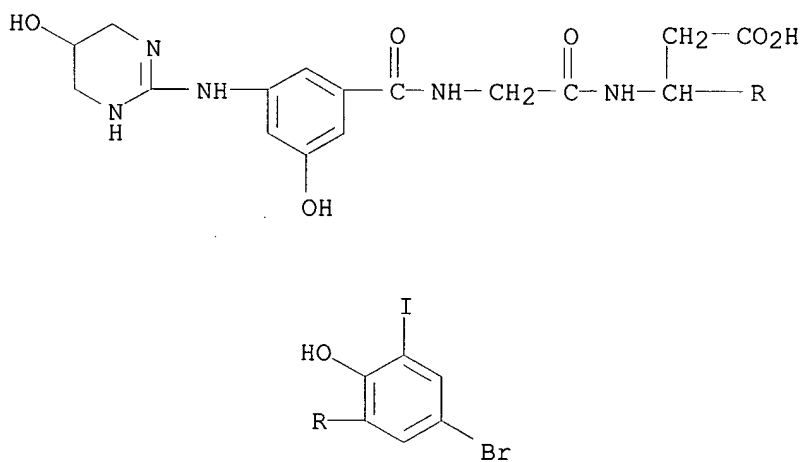
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-chloro-5-iodo-2-hydroxyphenyl)- (9CI)
MF C22 H23 Cl I N5 O7



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

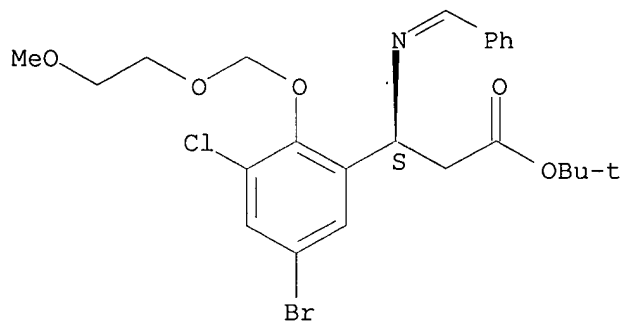
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-iodo-2-hydroxyphenyl)- (9CI)
MF C22 H23 Br I N5 O7



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

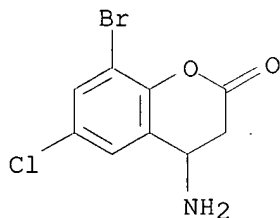
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzenepropanoic acid, 5-bromo-3-chloro-2-[(2-methoxyethoxy)methoxy]-.beta.-[(phenylmethylene)amino]-, 1,1-dimethylethyl ester, (.beta.S)- (9CI)
MF C24 H29 Br Cl N O5

Absolute stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

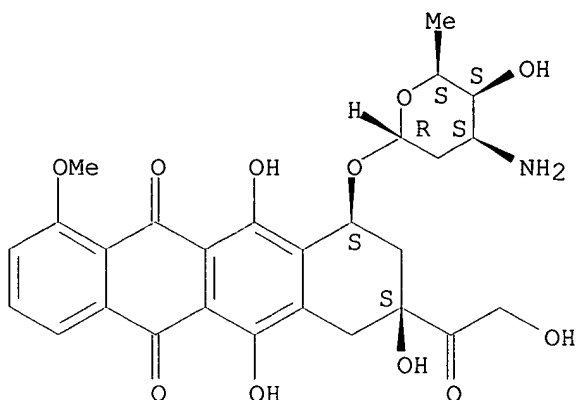
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2H-1-Benzopyran-2-one, 4-amino-8-bromo-6-chloro-3,4-dihydro-,
hydrochloride (9CI)
MF C9 H7 Br Cl N O2 . Cl H



● HCl

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 5,12-Naphthacenedione, 10-[(3-amino-2,3,6-trideoxy-.alpha.-L-lyxo-
hexopyranosyl)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(hydroxyacetyl)-
1-methoxy-, (8S,10S)- (9CI)
MF C27 H29 N O11
CI COM

Absolute stereochemistry.

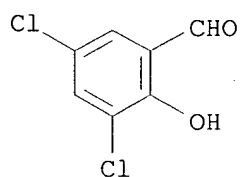


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Calcium (8CI, 9CI)
 MF Ca
 CI COM

Ca

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzaldehyde, 3,5-dichloro-2-hydroxy- (9CI)
 MF C7 H4 Cl2 O2
 CI COM

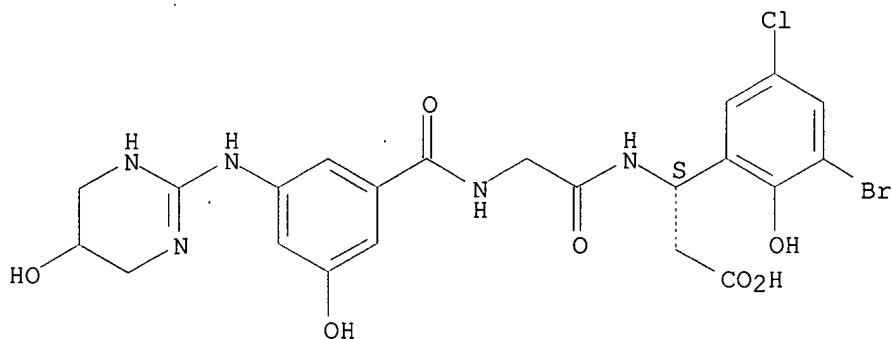


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

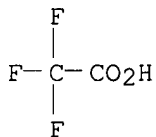
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3S)-, mono(trifluoroacetate) (salt) (9CI)
 MF C22 H23 Br Cl N5 O7 . C2 H F3 O2

CM 1

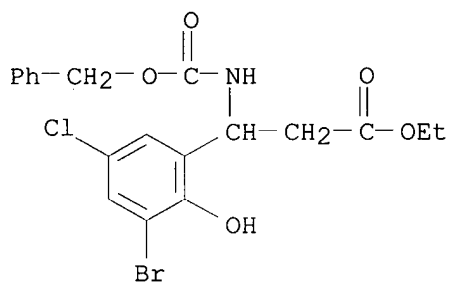
Absolute stereochemistry.



CM 2



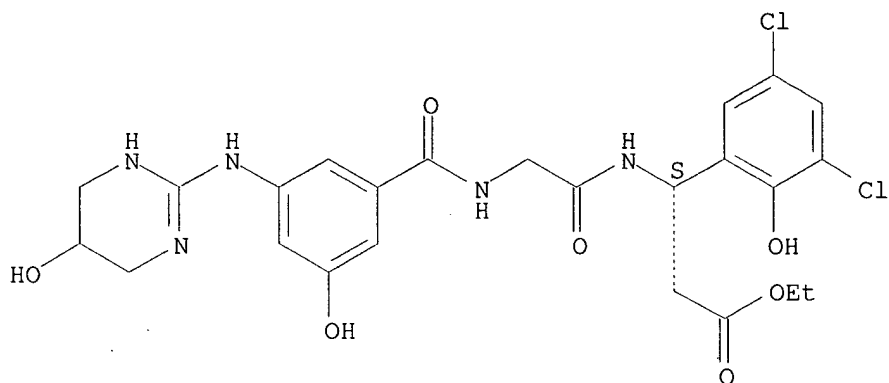
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzenepropanoic acid, 3-bromo-5-chloro-2-hydroxy-.beta.-
 [[(phenylmethoxy)carbonyl]amino]-, ethyl ester (9CI)
 MF C19 H19 Br Cl N O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-
 pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, ethyl
 ester, (3S)- (9CI)
 MF C24 H27 Cl2 N5 O7
 CI COM

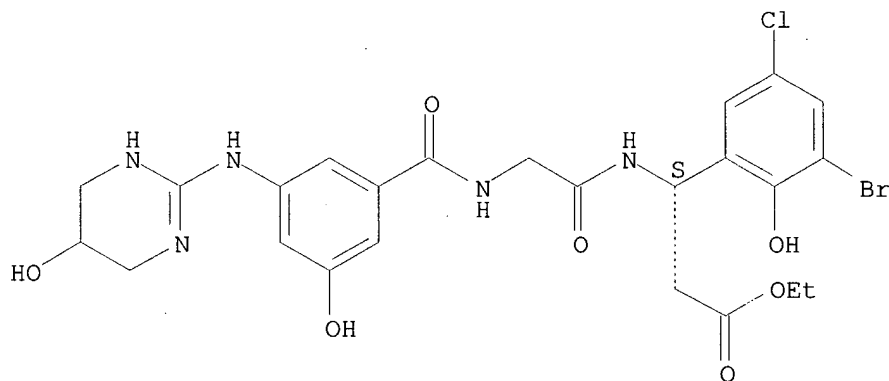
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, ethyl ester, (3S)- (9CI)
MF C24 H27 Br Cl N5 O7

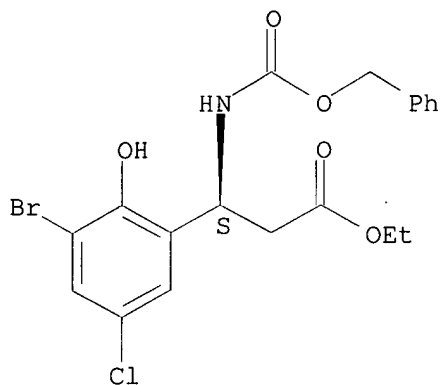
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

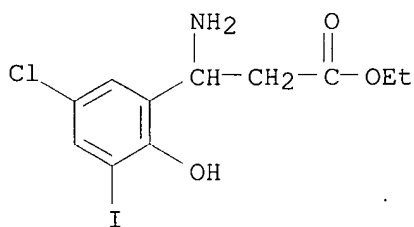
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzenepropanoic acid, 3-bromo-5-chloro-2-hydroxy-.beta.-[[[(phenylmethoxy)carbonyl]amino]-, ethyl ester, (.beta.S)- (9CI)
MF C19 H19 Br Cl N O5

Absolute stereochemistry.



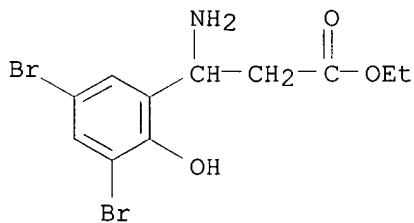
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzenepropanoic acid, .beta.-amino-5-chloro-2-hydroxy-3-iodo-, ethyl
ester, hydrochloride (9CI)
MF C11 H13 Cl I N O3 . Cl H



● HCl

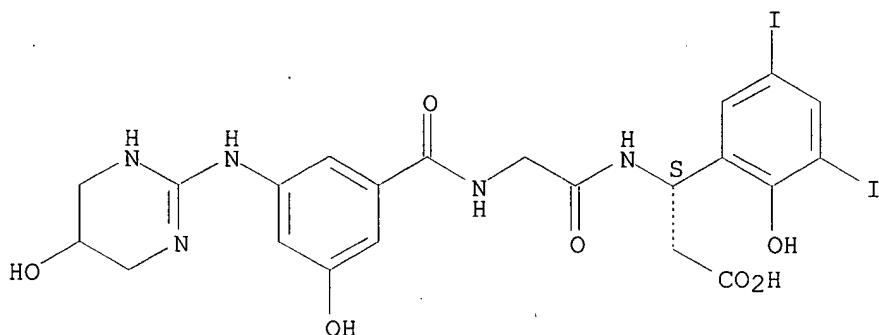
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzenepropanoic acid, .beta.-amino-3,5-dibromo-2-hydroxy-, ethyl ester,
hydrochloride (9CI)
MF C11 H13 Br2 N O3 . Cl H



● HCl

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-diiodo-2-hydroxyphenyl)-, (3S)-(9CI)
MF C22 H23 I2 N5 O7

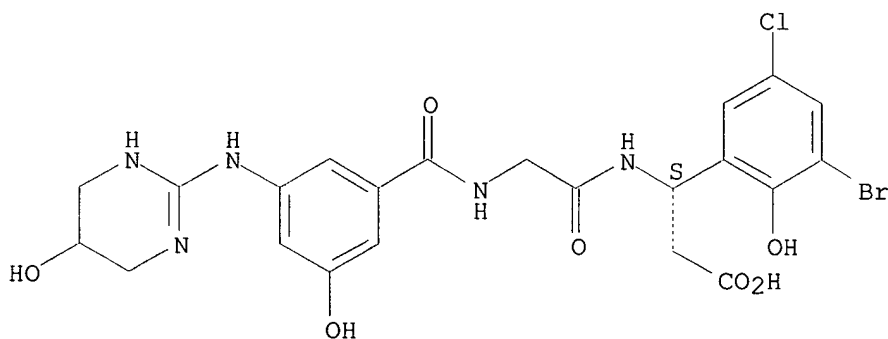
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

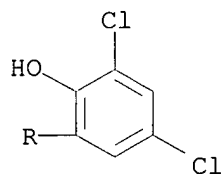
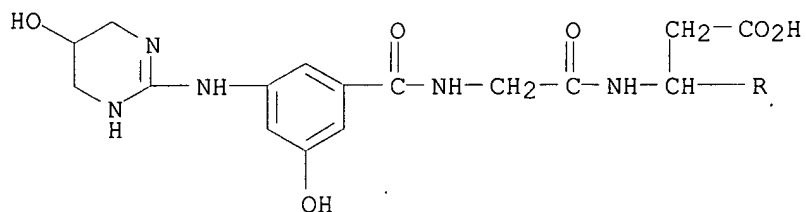
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3S)-(9CI)
MF C22 H23 Br Cl N5 O7
CI COM

Absolute stereochemistry.



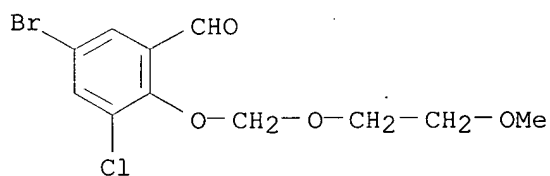
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)- (9CI)
MF C22 H23 Cl2 N5 O7



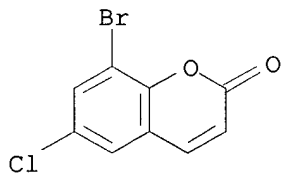
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzaldehyde, 5-bromo-3-chloro-2-[(2-methoxyethoxy)methoxy]- (9CI)
MF C11 H12 Br Cl O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

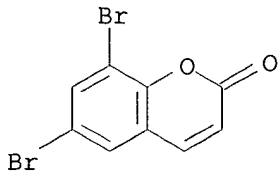
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2H-1-Benzopyran-2-one, 8-bromo-6-chloro- (9CI)
MF C9 H4 Br Cl O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

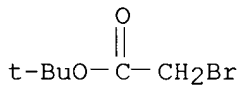
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2H-1-Benzopyran-2-one, 6,8-dibromo- (9CI)
MF C9 H4 Br2 O2



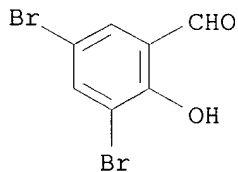
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Acetic acid, bromo-, 1,1-dimethylethyl ester (9CI)
MF C6 H11 Br O2
CI COM



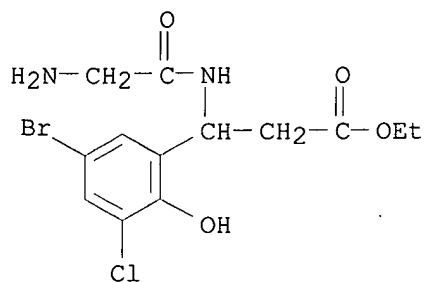
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzaldehyde, 3,5-dibromo-2-hydroxy- (9CI)
MF C7 H4 Br2 O2
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

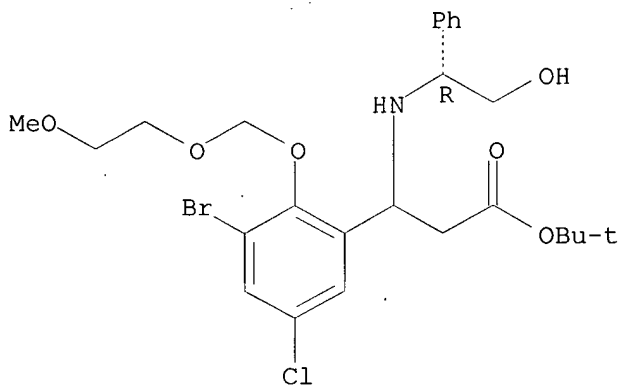
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, glycy-3-(5-bromo-3-chloro-2-hydroxyphenyl)-, ethyl ester,
monohydrochloride (9CI)
MF C13 H16 Br Cl N2 O4 . Cl H



● HCl

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzenepropanoic acid, 3-bromo-5-chloro-.beta.-[[(1R)-2-hydroxy-1-phenylethyl]amino]-2-[(2-methoxyethoxy)methoxy]-, 1,1-dimethylethyl ester (9CI)
MF C25 H33 Br Cl N O6

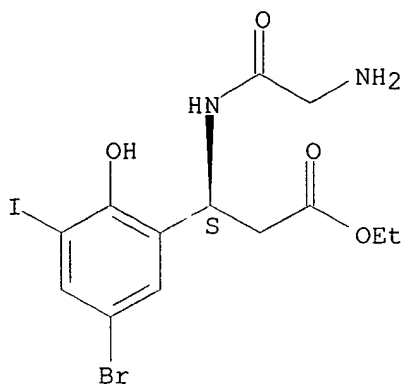
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, glycyl-3-(5-bromo-2-hydroxy-3-iodophenyl)-, ethyl ester, monohydrochloride (9CI)
MF C13 H16 Br I N2 O4 . Cl H

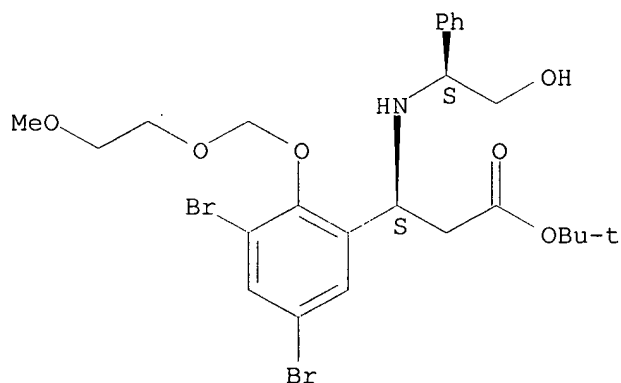
Absolute stereochemistry.



● HCl

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzenepropanoic acid, 3,5-dibromo-.beta.-[[(1S)-2-hydroxy-1-phenylethyl]amino]-2-[(2-methoxyethoxy)methoxy]-, 1,1-dimethylethyl ester, (.beta.S)- (9CI)
 MF C25 H33 Br2 N O6

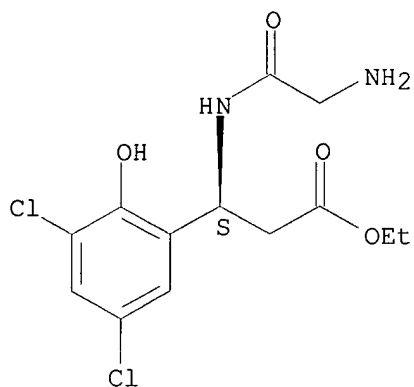
Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

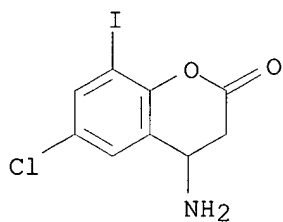
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN .beta.-Alanine, glycy-3-(3,5-dichloro-2-hydroxyphenyl)-, ethyl ester, monohydrochloride, (3S)- (9CI)
 MF C13 H16 Cl2 N2 O4 . Cl H

Absolute stereochemistry.



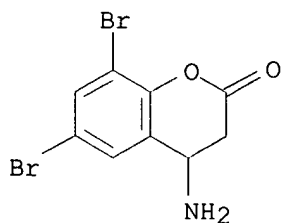
● HCl

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2H-1-Benzopyran-2-one, 4-amino-6-chloro-3,4-dihydro-8-iodo-, hydrochloride
(9CI)
MF C9 H7 Cl I N O2 . Cl H



● HCl

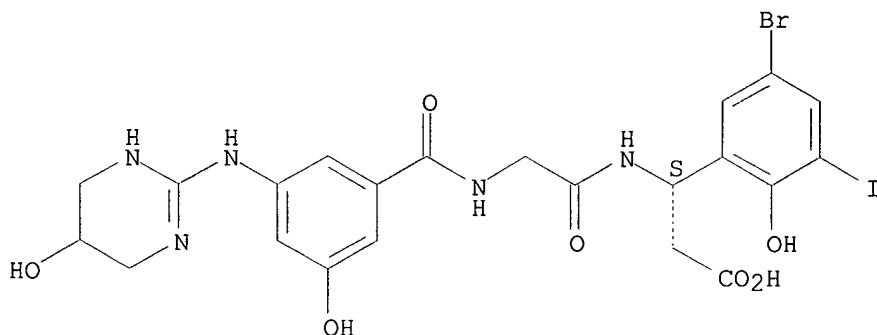
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2H-1-Benzopyran-2-one, 4-amino-6,8-dibromo-3,4-dihydro-, hydrochloride
(9CI)
MF C9 H7 Br2 N O2 . Cl H



● HCl

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-2-hydroxy-3-iodophenyl)-,
(3S)- (9CI)
MF C22 H23 Br I N5 O7
CI COM

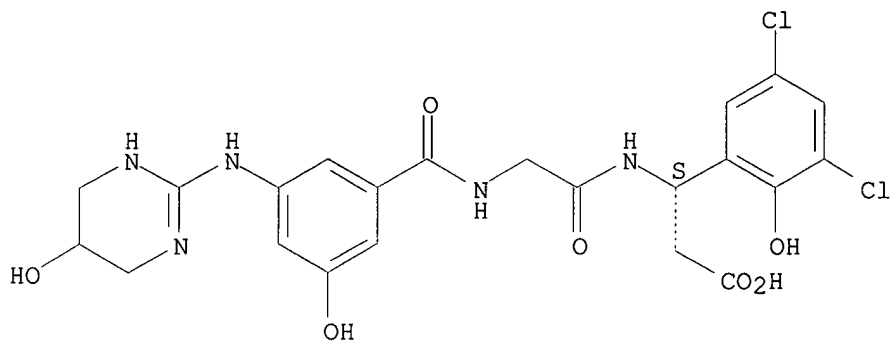
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

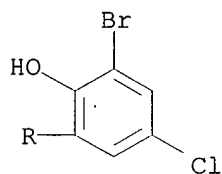
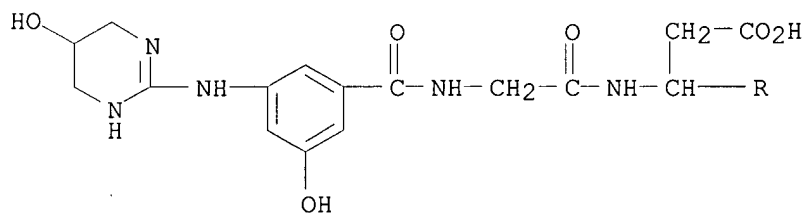
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-,
monohydrochloride, (3S)- (9CI)
MF C22 H23 Cl2 N5 O7 . Cl H

Absolute stereochemistry.



● HCl

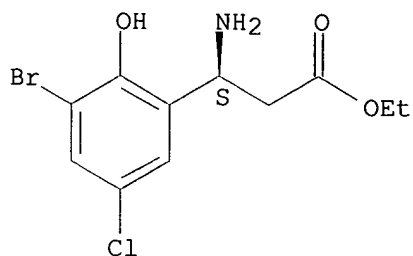
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-(9CI)
 MF C22 H23 Br Cl N5 O7
 CI COM



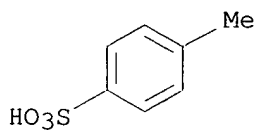
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzenepropanoic acid, .beta.-amino-3-bromo-5-chloro-2-hydroxy-, ethyl ester, (.beta.S)-, 4-methylbenzenesulfonate (salt) (9CI)
 MF C11 H13 Br Cl N O3 . C7 H8 O3 S
 CM 1

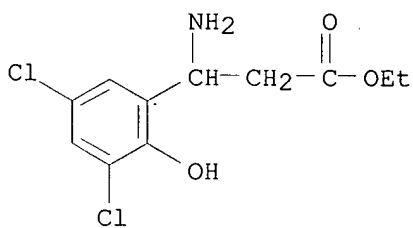
Absolute stereochemistry. Rotation (+).



CM 2



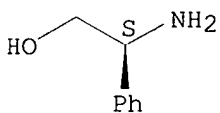
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzenepropanoic acid, .beta.-amino-3,5-dichloro-2-hydroxy-, ethyl ester,
hydrochloride (9CI)
MF C11 H13 Cl2 N O3 . Cl H



● HCl

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzeneethanol, .beta.-amino-, (.beta.S)- (9CI)
MF C8 H11 N O
CI COM

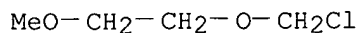
Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

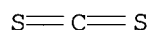
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Ethane, 1-(chloromethoxy)-2-methoxy- (7CI, 8CI, 9CI)
MF C4 H9 Cl O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Carbon disulfide (8CI, 9CI)
MF C S2
CI COM

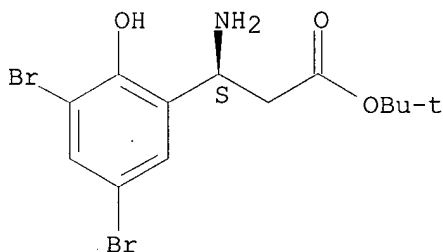


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

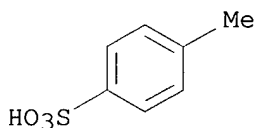
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzenepropanoic acid, .beta.-amino-3,5-dibromo-2-hydroxy-,
1,1-dimethylethyl ester, (.beta.S)-, 4-methylbenzenesulfonate (salt) (9CI)
MF C13 H17 Br2 N O3 . C7 H8 O3 S

CM 1

Absolute stereochemistry.

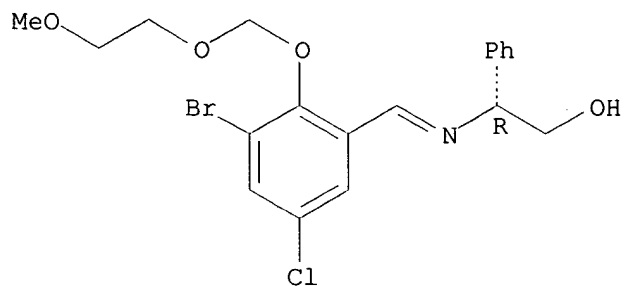


CM 2



L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzeneethanol, .beta.-[[[3-bromo-5-chloro-2-[(2-methoxyethoxy)methoxy]phenyl]methylene]amino]-, (.beta.R)- (9CI)
MF C19 H21 Br Cl N O4

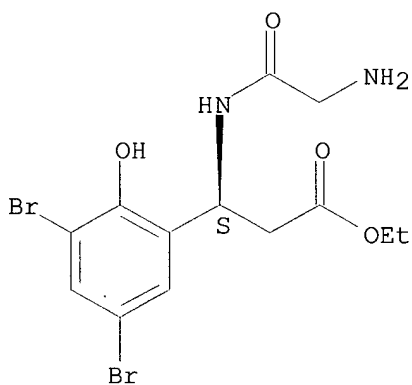
Absolute stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

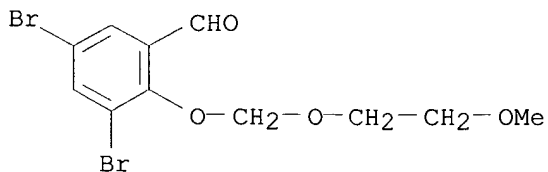
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, glycyI-3-(3,5-dibromo-2-hydroxyphenyl)-, ethyl ester,
monohydrochloride, (3S)- (9CI)
MF C13 H16 Br2 N2 O4 . Cl H

Absolute stereochemistry.



● HCl

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzaldehyde, 3,5-dibromo-2-[(2-methoxyethoxy)methoxy]- (9CI)
MF C11 H12 Br2 O4

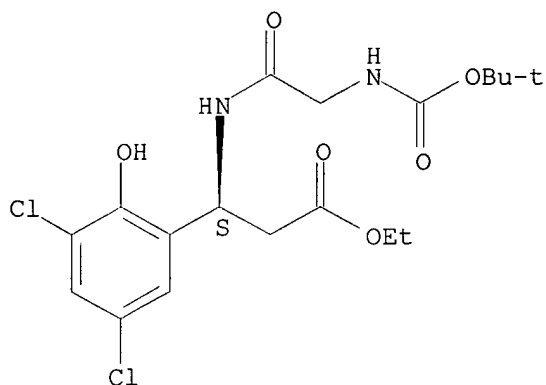


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS

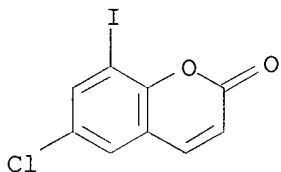
IN .beta.-Alanine, N-[(1,1-dimethylethoxy)carbonyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, ethyl ester, (3S)- (9CI)
MF C18 H24 Cl2 N2 O6

Absolute stereochemistry.



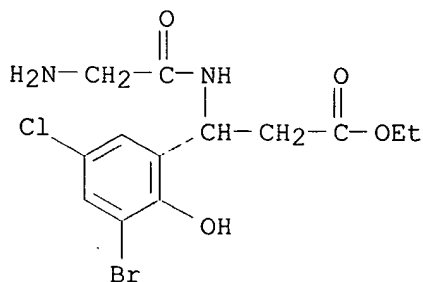
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2H-1-Benzopyran-2-one, 6-chloro-8-iodo- (9CI)
MF C9 H4 Cl I O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

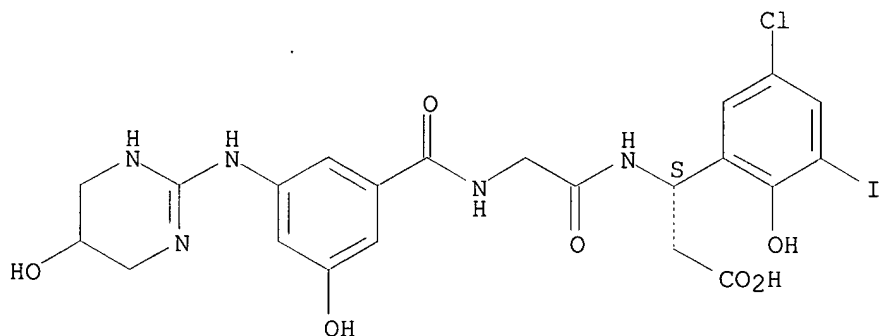
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, ethyl ester, monohydrochloride (9CI)
MF C13 H16 Br Cl N2 O4 . Cl H



● HCl

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-chloro-3-iodo-2-hydroxyphenyl)-,
(3S)- (9CI)
MF C22 H23 Cl I N5 O7

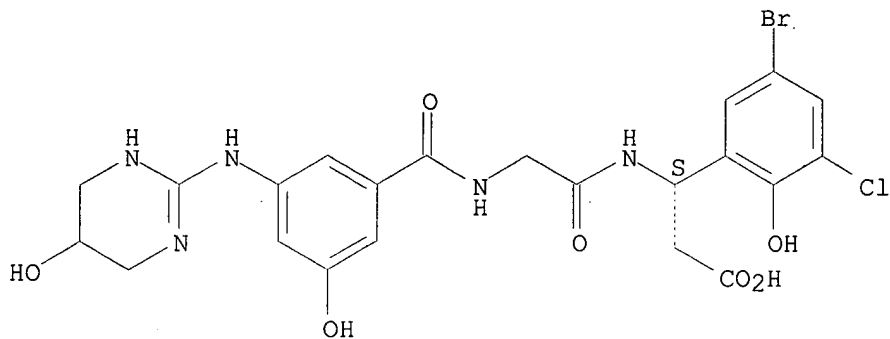
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)-,
(3S)- (9CI)
MF C22 H23 Br Cl N5 O7

Absolute stereochemistry.

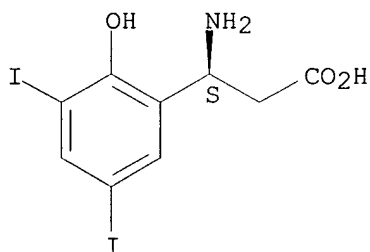


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

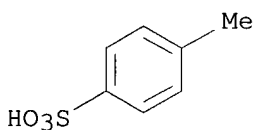
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzenepropanoic acid, .beta.-amino-2-hydroxy-3,5-diiodo-, (.beta.S)-,
 4-methylbenzenesulfonate (salt) (9CI)
 MF C9 H9 I2 N O3 . C7 H8 O3 S

CM 1

Absolute stereochemistry.

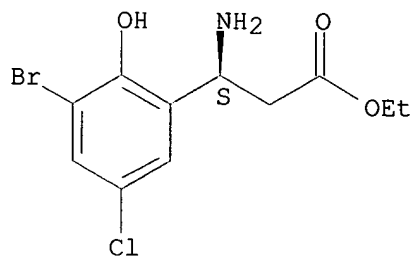


CM 2



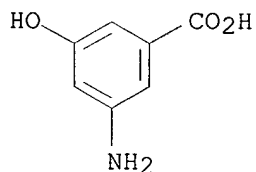
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzenepropanoic acid, .beta.-amino-3-bromo-5-chloro-2-hydroxy-, ethyl
 ester, (.beta.S)- (9CI)
 MF C11 H13 Br Cl N O3
 CI COM

Absolute stereochemistry. Rotation (+).



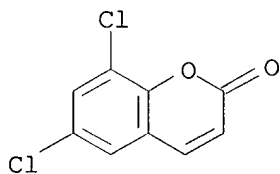
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 3-amino-5-hydroxy- (9CI)
MF C7 H7 N O3
CI COM



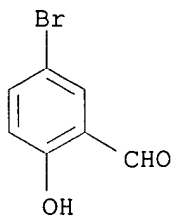
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2H-1-Benzopyran-2-one, 6,8-dichloro- (9CI)
MF C9 H4 Cl2 O2



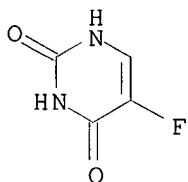
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzaldehyde, 5-bromo-2-hydroxy- (9CI)
MF C7 H5 Br O2
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

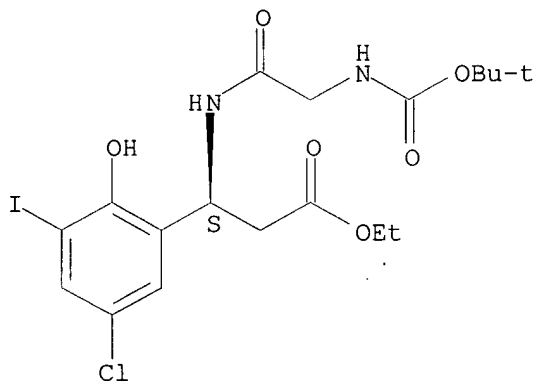
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro- (9CI)
MF C4 H3 F N2 O2
CI COM



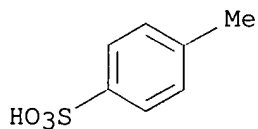
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, N-[(1,1-dimethylethoxy)carbonyl]glycyl-3-(5-chloro-3-iodo-2-hydroxyphenyl)-, ethyl ester, (3S)-, mono(4-methylbenzenesulfonate) (salt) (9CI)
MF C18 H24 Cl I N2 O6 . C7 H8 O3 S
CM 1

Absolute stereochemistry.

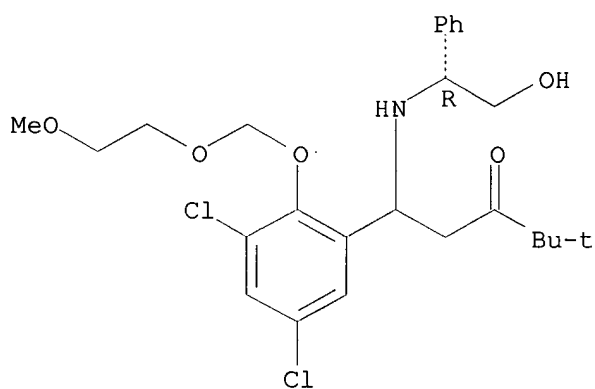


CM 2



L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 3-Pentanone, 1-[3,5-dichloro-2-[(2-methoxyethoxy)methoxy]phenyl]-1-[[(1R)-
2-hydroxy-1-phenylethyl]amino]-4,4-dimethyl- (9CI)
MF C25 H33 Cl2 N O5

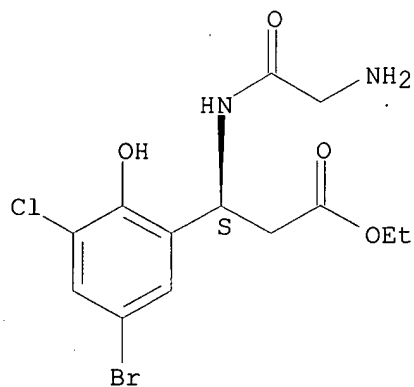
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)-, ethyl ester,
monohydrochloride, (3S)- (9CI)
MF C13 H16 Br Cl N2 O4 . Cl H

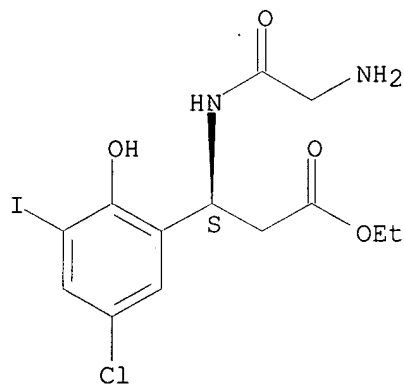
Absolute stereochemistry.



● HCl

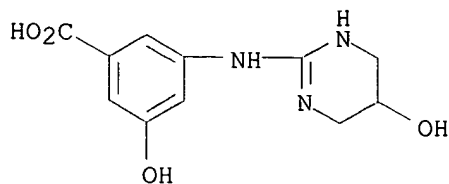
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, glycyl-3-(5-chloro-3-iodo-2-hydroxyphenyl)-, ethyl ester,
monohydrochloride, (3S)- (9CI)
MF C13 H16 Cl I N2 O4 . Cl H

Absolute stereochemistry.



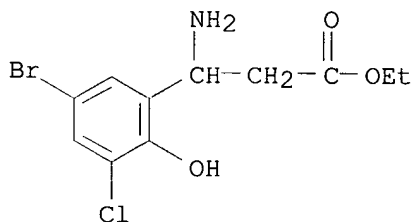
● HCl

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-
pyrimidinyl)amino]-, monohydrochloride (9CI)
MF C11 H13 N3 O4 . Cl H



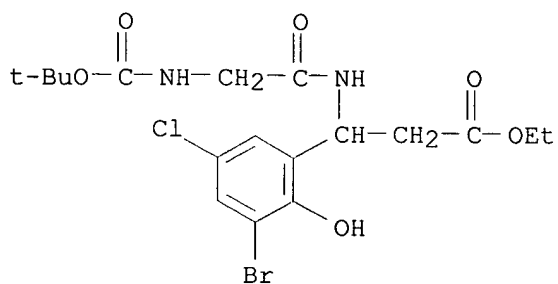
● HCl

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzenepropanoic acid, .beta.-amino-5-bromo-3-chloro-2-hydroxy-, ethyl
 ester, hydrochloride (9CI)
 MF C11 H13 Br Cl N O3 . Cl H



● HCl

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN .beta.-Alanine, N-[(1,1-dimethylethoxy)carbonyl]glycyl-3-(3-bromo-5-chloro-
 2-hydroxyphenyl)-, ethyl ester (9CI)
 MF C18 H24 Br Cl N2 O6

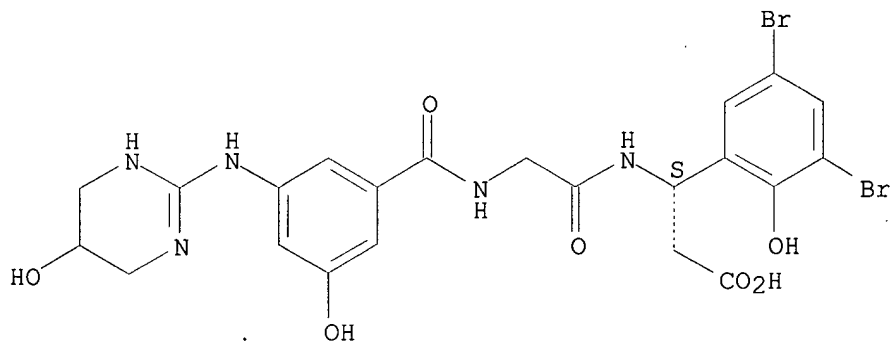


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS

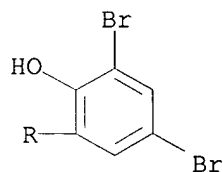
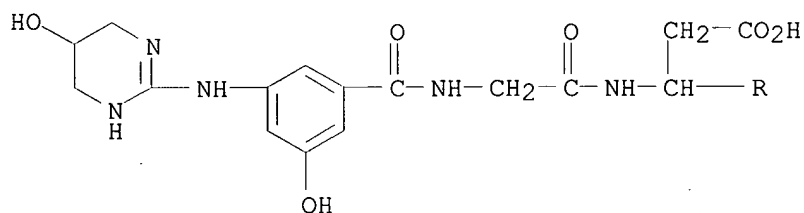
IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dibromo-2-hydroxyphenyl)-, (3S)-(9CI)
MF C22 H23 Br2 N5 O7
CI COM

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

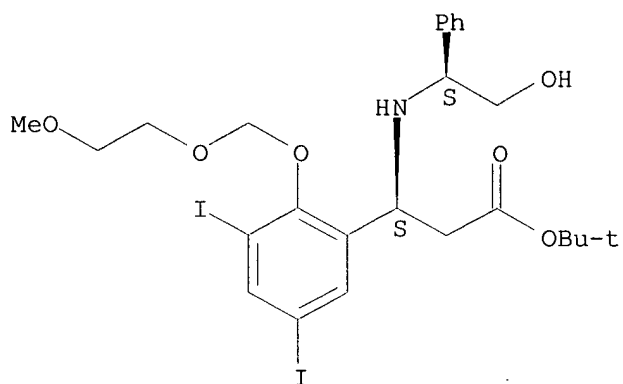
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dibromo-2-hydroxyphenyl)- (9CI)
MF C22 H23 Br2 N5 O7



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzenepropanoic acid, .beta.-[[(1S)-2-hydroxy-1-phenylethyl]amino]-3,5-diiodo-2-[(2-methoxyethoxy)methoxy]-, 1,1-dimethylethyl ester, (.beta.S)-(9CI)
MF C25 H33 I2 N O6

Absolute stereochemistry. Rotation (+).

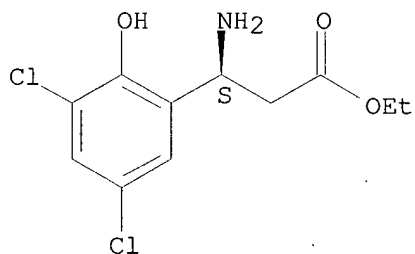


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

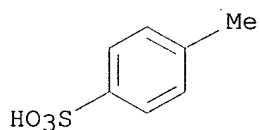
L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzenepropanoic acid, .beta.-amino-3,5-dichloro-2-hydroxy-, ethyl ester,
(.beta.S)-, 4-methylbenzenesulfonate (salt) (9CI)
MF C11 H13 Cl2 N O3 . C7 H8 O3 S

CM 1

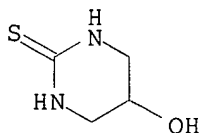
Absolute stereochemistry. Rotation (+).



CM 2

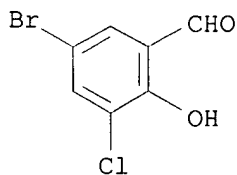


L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2(1H)-Pyrimidinethione, tetrahydro-5-hydroxy- (7CI, 9CI)
MF C4 H8 N2 O S



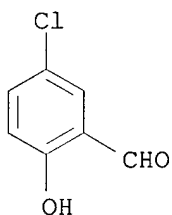
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzaldehyde, 5-bromo-3-chloro-2-hydroxy- (9CI)
MF C7 H4 Br Cl O2



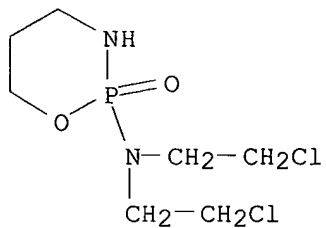
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzaldehyde, 5-chloro-2-hydroxy- (9CI)
MF C7 H5 Cl O2
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 104 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2H-1,3,2-Oxazaphosphorin-2-amine, N,N-bis(2-chloroethyl)tetrahydro-,
2-oxide (9CI)
MF C7 H15 Cl2 N2 O2 P
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> fil medl; d que l18; fil embase; d que l25

FILE 'MEDLINE' ENTERED AT 16:59:35 ON 17 MAR 2003

FILE LAST UPDATED: 16 MAR 2003 (20030316/UP). FILE COVERS 1958 TO DATE.

On June 9, 2002, MEDLINE was reloaded. See HELP RLOAD for details.

MEDLINE thesauri in the /CN, /CT, and /MN fields incorporate the MeSH 2003 vocabulary. See <http://www.nlm.nih.gov/mesh/summ2003.html> for a description on changes.

This file contains CAS Registry Numbers for easy and accurate substance identification.

L9 1152 SEA FILE=MEDLINE ABB=ON CUNNINGHAM J?/AU
L10 589 SEA FILE=MEDLINE ABB=ON GORDON G?/AU
L11 45 SEA FILE=MEDLINE ABB=ON NICKOLS G?/AU
L12 5 SEA FILE=MEDLINE ABB=ON RUMINSKI P?/AU
L13 23 SEA FILE=MEDLINE ABB=ON WESTLIN W?/AU
L14 448 SEA FILE=MEDLINE ABB=ON ROGERS T?/AU
L18 4 SEA FILE=MEDLINE ABB=ON (L9 AND (L10 OR L11 OR L12 OR L13 OR
(L14)) OR (L10 AND (L11 OR L12 OR L13 OR L14)) OR (L11 AND (L12
OR L13 OR L14)) OR (L12 AND (L13 OR L14)) OR (L13 AND L14)

*inventor
search
continued*

FILE 'EMBASE' ENTERED AT 16:59:35 ON 17 MAR 2003

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FILE COVERS 1974 TO 13 Mar 2003 (20030313/ED)

EMBASE has been reloaded. Enter HELP RLOAD for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

L19 1056 SEA FILE=EMBASE ABB=ON CUNNINGHAM J?/AU
L20 480 SEA FILE=EMBASE ABB=ON GORDON G?/AU
L21 48 SEA FILE=EMBASE ABB=ON NICKOLS G?/AU
L22 5 SEA FILE=EMBASE ABB=ON RUMINSKI P?/AU
L23 16 SEA FILE=EMBASE ABB=ON WESTLIN W?/AU
L24 404 SEA FILE=EMBASE ABB=ON ROGERS T?/AU
L25 4 SEA FILE=EMBASE ABB=ON (L19 AND (L20 OR L21 OR L22 OR L23 OR
L24)) OR (L20 AND (L21 OR L22 OR L23 OR L24)) OR (L21 AND (L22
OR L23 OR L24)) OR (L22 AND (L23 OR L24)) OR (L23 AND L24)

=> fil cancer; d que l32

FILE 'CANCERLIT' ENTERED AT 17:00:25 ON 17 MAR 2003

FILE COVERS 1963 TO 15 Nov 2002 (20021115/ED)

On July 28, 2002, CANCERLIT was reloaded. See HELP RLOAD for details.

CANCERLIT thesauri in the /CN, /CT, and /MN fields incorporate the MeSH 2002 vocabulary. Enter HELP THESAURUS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

L26 271 SEA FILE=CANCERLIT ABB=ON CUNNINGHAM J?/AU
L27 92 SEA FILE=CANCERLIT ABB=ON GORDON G?/AU
L28 10 SEA FILE=CANCERLIT ABB=ON NICKOLS G?/AU
L29 3 SEA FILE=CANCERLIT ABB=ON RUMINSKI P?/AU
L30 8 SEA FILE=CANCERLIT ABB=ON WESTLIN W?/AU
L31 86 SEA FILE=CANCERLIT ABB=ON ROGERS T?/AU
L32 3 SEA FILE=CANCERLIT ABB=ON (L26 AND (L27 OR L28 OR L29 OR L30
OR L31)) OR (L27 AND (L28 OR L29 OR L30 OR L31)) OR (L28 AND
(L29 OR L30 OR L31)) OR (L29 AND (L30 OR L31)) OR (L30 AND
L31).

=> dup rem 132,118,125

FILE 'CANCERLIT' ENTERED AT 17:00:43 ON 17 MAR 2003

FILE 'MEDLINE' ENTERED AT 17:00:43 ON 17 MAR 2003

FILE 'EMBASE' ENTERED AT 17:00:43 ON 17 MAR 2003

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PROCESSING COMPLETED FOR L32

PROCESSING COMPLETED FOR L18

PROCESSING COMPLETED FOR L25

L33 5 DUP REM L32 L18 L25 (6 DUPLICATES REMOVED)

ANSWERS '1-3' FROM FILE CANCERLIT

ANSWERS '4-5' FROM FILE MEDLINE

=> d ibib ab 1-5

L33 ANSWER 1 OF 5 CANCERLIT DUPLICATE 2
ACCESSION NUMBER: 2000224991 CANCERLIT
DOCUMENT NUMBER: 20224991 PubMed ID: 10763921
TITLE: Characterization of spontaneous metastasis in an aggressive
breast carcinoma model using flow cytometry.
AUTHOR: Schmidt C M; Settle S L; Keene J L; Westlin W F;
Nickols G A; Griggs D W
CORPORATE SOURCE: Searle Discovery Research, Monsanto Company, St. Louis,
Missouri 63198, USA.
SOURCE: CLINICAL AND EXPERIMENTAL METASTASIS, (1999) 17 (6) 537-44.
Journal code: 8409970. ISSN: 0262-0898.
PUB. COUNTRY: Netherlands
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: MEDLINE; Priority Journals
OTHER SOURCE: MEDLINE 2000224991
ENTRY MONTH: 200004
ENTRY DATE: Entered STN: 20000515
Last Updated on STN: 20000515

AB Studies of metastasis can be accelerated and provide more mechanistic
information using cell lines which reproducibly and aggressively
metastasize, and which are accurately and easily detected in tissues at
all stages of the metastatic process. Although reporter proteins such as
green fluorescent protein (GFP) and beta-galactosidase have improved the
tracking of tumor cells in vivo, their measurement has often been limited
to visual observation and manual counting. In this study, we exploited the
highly sensitive and objective quantitation provided by flow cytometry to
characterize, in detail, the sequence of events associated with orthotopic
metastasis in a highly aggressive mouse model. Following stable
transfection of the MDA-MB-435 breast carcinoma cell line with GFP, we
utilized an in vivo selection process to isolate a variant exhibiting
increased primary tumor growth and metastasis. As few as one fluorescent
tumor cell per 200,000 host cells could be accurately detected in
dissociated tissues by flow cytometry, allowing us to demonstrate that

metastatic cells migrate to the lungs of SCID mice very early after orthotopic implantation. Tumor burden in lungs increased in a smooth continuous manner, until death approximately eight weeks later. Levels of circulating tumor cells in blood were also detectable at an early timepoint, but remained relatively low throughout the course of secondary tumor development in the lungs. Surgical removal of the primary tumor at various times after inoculation significantly affected lung tumor burden, supporting the concept that circulating tumor cells in blood inefficiently initiate distal metastases. Furthermore, the continuing contribution to metastasis by the primary tumor was independent of tumor mass. The combined characteristics of enhanced orthotopic metastasis and quantitative detection in blood and tissues will make this a useful new model for the characterization of the multi-stage progression of cancer, and the preclinical evaluation of anti-neoplastic therapies.

L33 ANSWER 2 OF 5 CANCERLIT DUPLICATE 3
ACCESSION NUMBER: 1998240991 CANCERLIT
DOCUMENT NUMBER: 98240991 PubMed ID: 9581835
TITLE: A peptidomimetic antagonist of the integrin alpha(v)beta3 inhibits Leydig cell tumor growth and the development of hypercalcemia of malignancy.
AUTHOR: Carron C P; Meyer D M; Pegg J A; Engleman V W; Nickols M A; Settle S L; Westlin W F; Ruminski P G; Nickols G A
CORPORATE SOURCE: Department of Discovery Pharmacology, Searle Research and Development, Monsanto Company, St. Louis, Missouri 63198, USA.. cpcarr@monsanto.com
SOURCE: CANCER RESEARCH, (1998 May 1) 58 (9) 1930-5.
Journal code: 2984705R. ISSN: 0008-5472.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: MEDLINE; Priority Journals
OTHER SOURCE: MEDLINE 1998240991
ENTRY MONTH: 199806
ENTRY DATE: Entered STN: 19980713
Last Updated on STN: 19980713

AB The integrin alpha(v)beta3 interacts with the arginine-glycine-aspartic acid (RGD) tripeptide recognition sequence of a variety of extracellular matrix proteins. Recent studies show that alpha(v)beta3 plays an important role in tumor-induced angiogenesis and tumor growth and that antagonists of alpha(v)beta3 inhibit angiogenic processes that include endothelial cell adhesion and migration. Consequently, we reasoned that an RGD-based peptidomimetic antagonist of alpha(v)beta3 might inhibit tumor angiogenesis and tumor growth in vivo. An RGD-peptidomimetic library was screened to identify antagonists of vitronectin binding to alpha(v)beta3, and the compounds chosen were modified to produce selective and potent inhibitors of alpha(v)beta3. One of these compounds, beta-[[2-[[[3-[(aminoiminomethyl)amino]-phenyl]carbonyl]amino]acetyl]amino]-3,5-dichlorobenzenepropanoic acid (SC-68448), inhibited vitronectin binding to both alpha(v)beta3 and the closely related platelet receptor, alpha(IIb)beta3, in a dose-responsive manner. SC-68448 inhibited vitronectin binding to alpha(v)beta3 (IC50, 1 nM) and fibrinogen binding to the platelet receptor alpha(IIb)beta3 (IC50, >100 nM), demonstrating that SC-68448 was 100-fold more potent as an inhibitor of alpha(v)beta3 versus alpha(IIb)beta3. In cell-based studies, SC-68448 inhibited alpha(v)beta3-mediated endothelial cell proliferation in a dose-dependent manner but did not inhibit tumor cell proliferation, suggesting that effects on endothelial cell proliferation were not due to SC-68448-induced cytotoxicity. In accord with these results, SC-68448 inhibited angiogenesis in vivo in a basic fibroblast growth factor-induced rat corneal neovascularization model. A xenogeneic severe combined immune deficiency mouse/rat Leydig cell tumor model was developed for testing

SC-68448 as an inhibitor of tumor growth in vivo. Rat Leydig cell tumors grew rapidly in severe combined immune deficiency mice and produced humoral hypercalcemia of malignancy. SC-68448 inhibited the growth of the tumors in mice by up to 80% and completely blocked the development of hypercalcemia. Together, these results demonstrate the feasibility of antitumor therapies based upon the development of nontoxic small molecule pharmacological antagonists of integrin alpha(v)beta3.

L33 ANSWER 3 OF 5 CANCERLIT
ACCESSION NUMBER: 1998638389 CANCERLIT
DOCUMENT NUMBER: 98638389
TITLE: Antiangiogenic and anticancer activities of antagonists of integrin alphavbeta3 (Meeting abstract).
AUTHOR: Nickols A; **Westlin W**; Meyer D; Pegg J; Engleman W; **Ruminski P**; Nickols M; Settle S; Carron C
CORPORATE SOURCE: Searle/Monsanto, St. Louis, MO 63167.
SOURCE: Proc Annu Meet Am Assoc Cancer Res, (1997) 38 A1389.
ISSN: 0197-016X.
DOCUMENT TYPE: (MEETING ABSTRACTS)
LANGUAGE: English
FILE SEGMENT: Institute for Cell and Developmental Biology
ENTRY MONTH: 199801
ENTRY DATE: Entered STN: 19980109
Last Updated on STN: 19980109

AB The integrin alphavbeta3 is utilized by endothelial cells during the process of angiogenesis. We hypothesized that antagonists of alphavbeta3 would disrupt the angiogenic process, resulting in impaired tumor growth and reduced metastasis. An antibody to alphavbeta3 (11D2) and a small molecule, peptidomimetic antagonist of alphavbeta3 (compound S448) were evaluated in several models of angiogenesis and tumor growth. S448 inhibited binding of vitronectin to purified, human alphavbeta3 dose dependently with an IC50 of 10nM. The attachment of M21 human melanoma cells to purified matrix proteins was inhibited by the alphavbeta3 antagonists. Both 11D2 and S448 prevented the proliferation of human microvessel endothelial cells on vitronectin and osteopontin in a dose dependent manner. In the chick CAM assay of angiogenesis, S448 and 11D2 both inhibited new blood vessel formation in response to bFGF. Additionally, the antagonists of alphavbeta3 impaired angiogenesis to bFGF in the mouse corneal micropocket model. Rice Leydig tumor cells grew rapidly and formed highly vascularized tumors when implanted SQ in SCID mice. S448 impaired tumor growth in a dose dependent manner with a maximal inhibitory response of 80%. S448 also prevented the humoral hypercalcemia of malignancy associated with this model. These results indicate that antagonists of integrin alphavbeta3 are potent inhibitors of angiogenesis and thus, offer a powerful new tool for the treatment of solid tumors.

L33 ANSWER 4 OF 5 MEDLINE DUPLICATE 1
ACCESSION NUMBER: 2000413850 MEDLINE
DOCUMENT NUMBER: 20291175 PubMed ID: 10828842
TITLE: Peptidomimetic antagonists of alphavbeta3 inhibit bone resorption by inhibiting osteoclast bone resorptive activity, not osteoclast adhesion to bone.
AUTHOR: Carron C P; Meyer D M; Engleman V W; Rico J G; **Ruminski P G**; Ornberg R L; **Westlin W F**; **Nickols G A**
CORPORATE SOURCE: Departments of Discovery Pharmacology, Medicinal Chemistry and Oncology, Searle Research and Development, Monsanto Company, St Louis, Missouri, 63198, USA..
SOURCE: chris.p.carron@monsanto.com
JOURNAL OF ENDOCRINOLOGY, (2000 Jun) 165 (3) 587-98.
Journal code: 0375363. ISSN: 0022-0795.
PUB. COUNTRY: ENGLAND: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200008
ENTRY DATE: Entered STN: 20000907
Last Updated on STN: 20000907
Entered Medline: 20000829

AB Osteoclasts are actively motile on bone surfaces and undergo alternating cycles of migration and resorption. Osteoclast interaction with the extracellular matrix plays a key role in the osteoclast resorptive process and a substantial body of evidence suggests that integrin receptors are important in osteoclast function. These integrin receptors bind to the Arg-Gly-Asp (RGD) sequence found in a variety of extracellular matrix proteins and it is well established that the interaction of osteoclast alpha v beta 3 integrin with the RGD motif within bone matrix proteins is important in osteoclast-mediated bone resorption. In this study, we characterized the effects of two synthetic peptidomimetic antagonists of alpha v beta 3, SC-56631 and SC-65811, on rabbit osteoclast adhesion to purified matrix proteins and bone, and on bone resorption in vitro. SC-56631 and SC-65811 are potent inhibitors of vitronectin binding to purified alpha v beta 3. Both SC-56631 and SC-65811 inhibited osteoclast adhesion to osteopontin- and vitronectin-coated surfaces and time-lapse video microscopy showed that osteoclasts rapidly retract from osteopontin-coated surfaces when exposed to SC-56631 and SC-65811. SC-56631 and SC-65811 blocked osteoclast-mediated bone resorption in a dose-responsive manner. Further analysis showed that SC-65811 and SC-56631 reduced the number of resorption pits produced per osteoclast and the average pit size. SC-65811 was a more potent inhibitor of bone resorption and the combination of reduced pit number and size led to a 90% inhibition of bone resorption. Surprisingly, however, osteoclasts treated with SC-65811, SC-56631 or the disintegrin echistatin, at concentrations that inhibit bone resorption did not inhibit osteoclast adhesion to bone. These results suggest that alphavbeta3 antagonists inhibited bone resorption by decreasing osteoclast bone resorptive activity or efficiency but not by inhibiting osteoclast adhesion to bone per se.

L33 ANSWER 5 OF 5 MEDLINE DUPLICATE 4
ACCESSION NUMBER: 97296219 MEDLINE
DOCUMENT NUMBER: 97296219 PubMed ID: 9151803
TITLE: A peptidomimetic antagonist of the alpha(v)beta3 integrin inhibits bone resorption in vitro and prevents osteoporosis in vivo.
COMMENT: Comment in: J Clin Invest. 1997 May 1;99(9):2059
AUTHOR: Engleman V W; Nickols G A; Ross F P; Horton M A; Griggs D W; Settle S L; Ruminski P G; Teitelbaum S L
CORPORATE SOURCE: Searle Corporation, St. Louis, Missouri 63167, USA.
CONTRACT NUMBER: AR32788 (NIAMS)
AR42404 (NIAMS)
DE05413 (NIDCR)
SOURCE: JOURNAL OF CLINICAL INVESTIGATION, (1997 May 1) 99 (9) 2284-92.
Journal code: 7802877. ISSN: 0021-9738.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Abridged Index Medicus Journals; Priority Journals
ENTRY MONTH: 199706
ENTRY DATE: Entered STN: 19970709
Last Updated on STN: 20021227
Entered Medline: 19970624

AB Osteoclastic bone degradation requires intimacy between the matrix and the resorptive cell. While the precise role the integrin alpha(v)beta3 plays in the process is not yet understood, occupancy of the heterodimer by

soluble ligand or by blocking antibody effectively inhibits bone resorption in vitro and in vivo, suggesting that $\alpha(v)\beta3$ blockade may prevent postmenopausal osteoporosis. Thus, we identified a synthetic chemical peptide mimetic, β -[2-[[5-[(aminoiminomethyl)amino]-1-oxopentyl]amino]-1-+ ++oxoethyl]amino-3-pyridinepropanoic acid, bistrifluoroacetate (SC56631) based upon the $\alpha(v)\beta3$ ligand, Arg-Gly-Asp (RGD), which recognizes the isolated integrin, and its relative, $\alpha(v)\beta5$, as effectively as does the natural peptide. The mimetic dampens osteoclastic bone resorption in vitro and in vivo. Most importantly, intravenous administration of the mimetic prevents the 55% loss of trabecular bone sustained by rats within 6 wk of oophorectomy. Histological examination of bones taken from SC56631-treated, oophorectomized animals also demonstrates the compound's bone sparing properties and its capacity to decrease osteoclast number. Thus, an RGD mimetic prevents the rapid bone loss that accompanies estrogen withdrawal.

=> fil reg; d stat que 136

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DICTIONARY FILE UPDATES: 16 MAR 2003 HIGHEST RN 499182-00-2

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

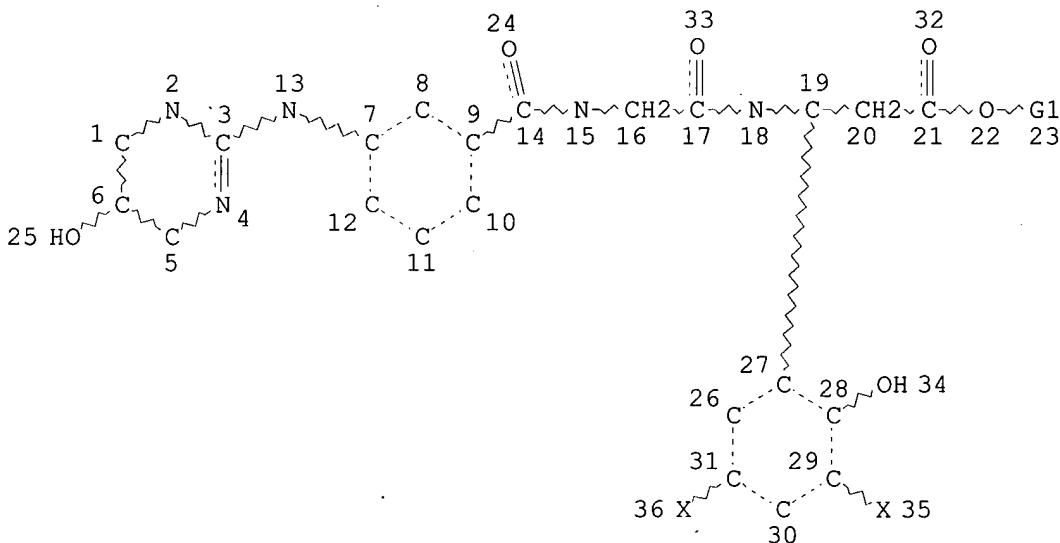
Please note that search-term pricing does apply when
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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

L34

STR



Ak @37

X = any halogen

VAR G1=H/37

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 37

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 37

STEREO ATTRIBUTES: NONE

L36 36 SEA FILE=REGISTRY SSS FUL L34

100.0% PROCESSED 550 ITERATIONS
SEARCH TIME: 00.00.01

36 ANSWERS

=> fil capl; d que nos 145; d que nos 155

FILE 'CAPLUS' ENTERED AT 17:18:29 ON 17 MAR 2003
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FILE COVERS 1907 - 17 Mar 2003 VOL 138 ISS 12
FILE LAST UPDATED: 16 Mar 2003 (20030316/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

L34 STR
L36 36 SEA FILE=REGISTRY SSS FUL L34
L37 1 SEA FILE=REGISTRY ABB=ON TAXOL/CN
L38 1 SEA FILE=REGISTRY ABB=ON CISPLATIN/CN
L39 1 SEA FILE=REGISTRY ABB=ON CYCLOPHOSPHAMIDE/CN
L40 3 SEA FILE=REGISTRY ABB=ON 5-FLUOROURACIL/CN OR "5-FLUOROURACIL LITHIUM SALT"/CN OR "5-FLUOROURACIL MONOSODIUM SALT"/CN
L41 1 SEA FILE=REGISTRY ABB=ON DOXORUBICIN/CN
L42 14 SEA FILE=CAPLUS ABB=ON L36
L43 46085 SEA FILE=CAPLUS ABB=ON (L37 OR L38 OR L39 OR L40 OR L41)
L44 49118 SEA FILE=CAPLUS ABB=ON TAXOL OR CISPLATIN OR CYCLOPHOSPHAMIDE OR FLUOROURACIL OR DOXORUBICIN
L45 6 SEA FILE=CAPLUS ABB=ON L42 AND (L43 OR L44)

L34 STR
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L42 14 SEA FILE=CAPLUS ABB=ON L36
L46 151708 SEA FILE=CAPLUS ABB=ON ANTITUMOR AGENTS+OLD/CT
L47 272118 SEA FILE=CAPLUS ABB=ON NEOPLAS?/CW
L51 52304 SEA FILE=CAPLUS ABB=ON COMBINATION#/OBI
L55 7 SEA FILE=CAPLUS ABB=ON L42 AND (L46 OR L47) AND L51

=> s 145 or 155

L63 8 L45 OR L55

=> fil uspatf; d que nos 161

FILE 'USPATFULL' ENTERED AT 17:18:30 ON 17 MAR 2003
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FILE COVERS 1971 TO PATENT PUBLICATION DATE: 13 Mar 2003 (20030313/PD)
FILE LAST UPDATED: 13 Mar 2003 (20030313/ED)
HIGHEST GRANTED PATENT NUMBER: US6532593
HIGHEST APPLICATION PUBLICATION NUMBER: US2003051284
CA INDEXING IS CURRENT THROUGH 13 Mar 2003 (20030313/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 13 Mar 2003 (20030313/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2002
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2002

>>> USPAT2 is now available. USPATFULL contains full text of the <<<
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>>> classifications, or claims, that may potentially change from <<<
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substance identification.

L34 STR
L36 36 SEA FILE=REGISTRY SSS FUL L34
L37 1 SEA FILE=REGISTRY ABB=ON TAXOL/CN
L38 1 SEA FILE=REGISTRY ABB=ON CISPLATIN/CN
L39 1 SEA FILE=REGISTRY ABB=ON CYCLOPHOSPHAMIDE/CN
L40 3 SEA FILE=REGISTRY ABB=ON 5-FLUOROURACIL/CN OR "5-FLUOROURACIL
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L57 5 SEA FILE=USPATFULL ABB=ON L36
L58 17387 SEA FILE=USPATFULL ABB=ON ANTITUMOR AGENTS/CT OR NEOPLASM
INHIBITORS/CT
L59 2855 SEA FILE=USPATFULL ABB=ON (L37 OR L38 OR L39 OR L40 OR L41)
L60 3008 SEA FILE=USPATFULL ABB=ON (TAXOL OR CISPLATIN OR CYCLOPHOSPHAM
IDE OR FLUOROURACIL OR DOXORUBICIN)/IT, TI, AB, CLM
L61 3 SEA FILE=USPATFULL ABB=ON L57 AND (L58 OR L59 OR L60)

=> dup rem 163,161

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PROCESSING COMPLETED FOR L63

PROCESSING COMPLETED FOR L61
COMMAND INTERRUPTED

=> dup rem 163,161

PROCESSING COMPLETED FOR L63

PROCESSING COMPLETED FOR L61

L65 10 DUP REM L63 L61 (1 DUPLICATE REMOVED)

ANSWERS '1-8' FROM FILE CAPLUS

ANSWERS '9-10' FROM FILE USPATFULL

=> d ibib abs hitstr 1-10'

L65 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2003 ACS DUPLICATE 1

ACCESSION NUMBER: 2002:290790 CAPLUS

DOCUMENT NUMBER: 136:310191

TITLE: Preparation of peptidyl integrin antagonists for use
in **combination** with a chemotherapeutic agent
for treatment of neoplasia

INVENTOR(S): Cunningham, Jay; Gordon, Gary B.; Nickols, G. Allen;
Westlin, William F.; Rogers, Thomas Edward; Ruminski,
Peter Gerrard

PATENT ASSIGNEE(S): USA

SOURCE: U.S., 35 pp., Cont.-in-part of U.S. Ser. No. 34,270,
abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

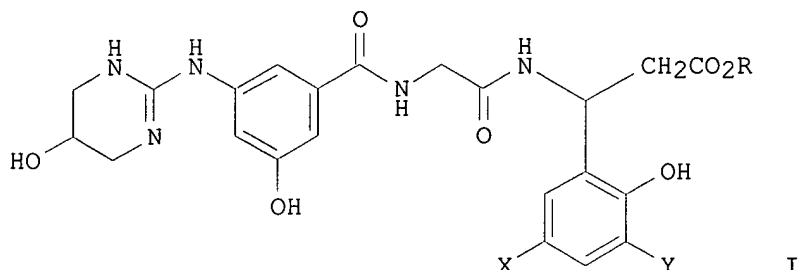
FAMILY ACC. NUM. COUNT: 5

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6372719	B1	20020416	US 1999-262725	19990304
ZA 9904406	A	20000211	ZA 1999-4406	19990211
WO 2000051686	A1	20000908	WO 2000-US3705	20000301
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
EP 1161280	A1	20011212	EP 2000-914580	20000301
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
JP 2002538177	T2	20021112	JP 2000-602347	20000301
US 2003050250	A1	20030313	US 2001-16146	20011210
PRIORITY APPLN. INFO.:			US 1998-34270	B2 19980304
			US 1999-262725	A 19990304
			WO 2000-US3705	W 20000301

OTHER SOURCE(S): MARPAT 136:310191

GI



- AB Peptides I (R = H, alkyl; X, Y = halo) were prepd. as .alpha.v.beta.3 integrin antagonists which in combination with a chemotherapeutic agent (**cisplatin**, **cyclophosphamide**, **5-fluorouracil**, **doxorubicin** and **taxol**) are used for treatment of neoplasia. Thus, 3-bromo-5-chloro-2-hydroxy-.beta.-[[2-[[[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxypyrimidin-2-yl)amino]phenyl]carbonyl]amino]acetyl]amino]benzenepropanoic acid trifluoroacetate was prepd. by peptide coupling of N-glycyl-.beta.-(3-bromo-5-chloro-2-hydroxyphenyl)-.beta.-aminopropionic acid Et ester with 3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxypyrimidin-2-yl)amino]benzoic acid. Peptides I delayed the growth of tumors in mice, particularly when combined with a chemotherapeutic agent.
- IT **243135-63-9P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)- **243135-65-1P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)- **243135-66-2P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-iodo-2-hydroxyphenyl)- **243135-67-3P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)- **243135-68-4P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-chloro-3-iodo-2-hydroxyphenyl)- **243135-69-5P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dibromo-2-hydroxyphenyl)- **243135-70-8P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)-, (3S)- **243135-71-9P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, monohydrochloride, (3S)- **243135-72-0P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3S)- **243135-74-2P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-chloro-5-iodo-2-hydroxyphenyl)- **243135-75-3P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-iodo-2-hydroxyphenyl)- **243135-76-4P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-diiodo-2-hydroxyphenyl)- **243135-78-6P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dibromo-2-hydroxyphenyl)-, (3S)- **243135-79-7P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-chloro-3-iodo-2-hydroxyphenyl)-, (3S)- **243135-80-0P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-2-hydroxy-3-iodophenyl)-,

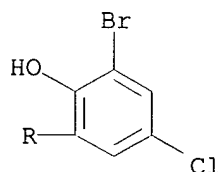
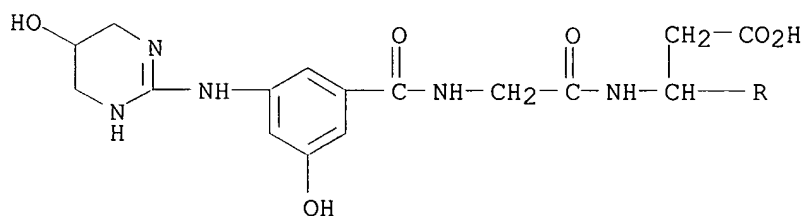
(3S)- **243135-81-1P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-diiodo-2-hydroxyphenyl)-, (3S)- **290826-47-0P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, compd. with trifluoromethanol

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptidyl integrin antagonists for use in **combination** with a chemotherapeutic agent for treatment of neoplasia)

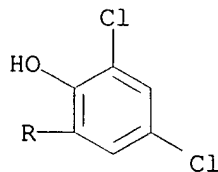
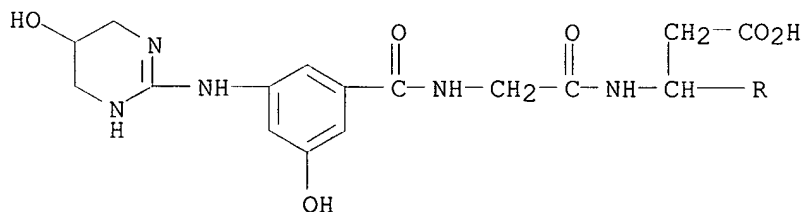
RN 243135-63-9 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-(9CI) (CA INDEX NAME)



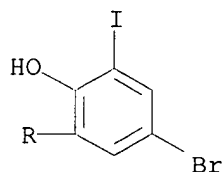
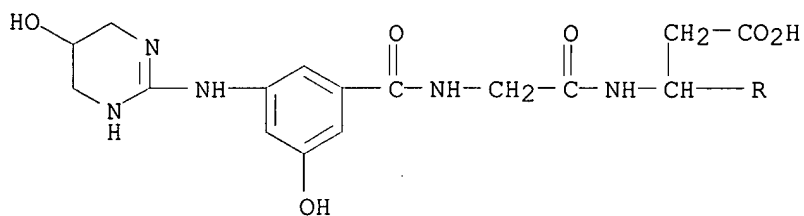
RN 243135-65-1 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-(9CI) (CA INDEX NAME)



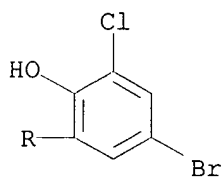
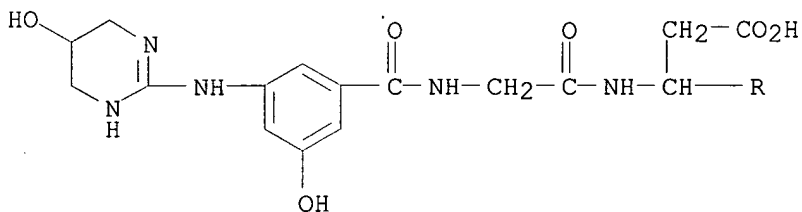
RN 243135-66-2 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-iodo-2-hydroxyphenyl)-(9CI) (CA INDEX NAME)



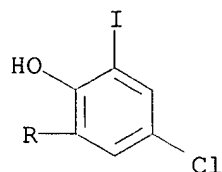
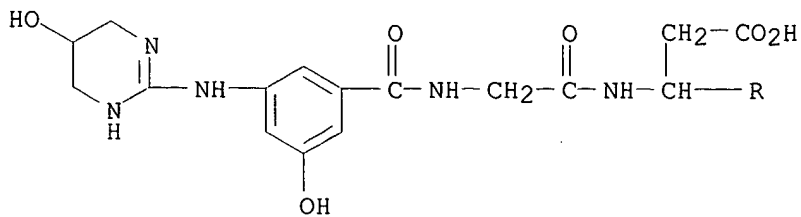
RN 243135-67-3 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)-
(9CI) (CA INDEX NAME)



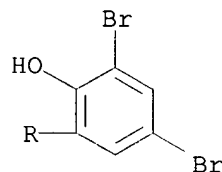
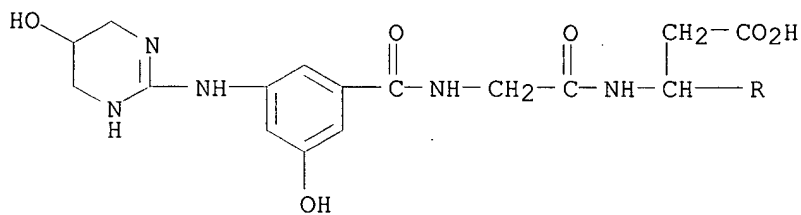
RN 243135-68-4 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-chloro-3-iodo-2-hydroxyphenyl)-
(9CI) (CA INDEX NAME)



RN 243135-69-5 CAPLUS

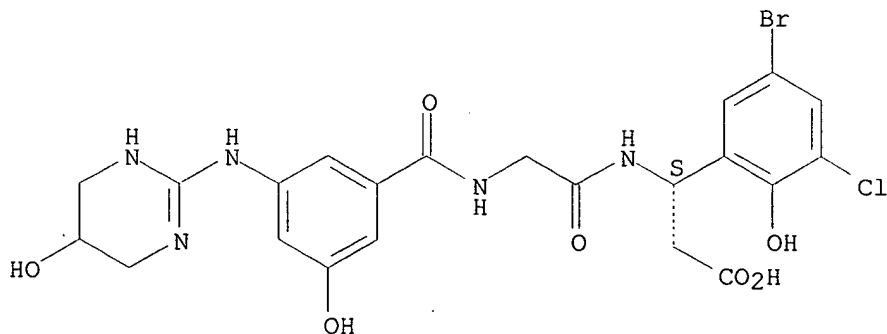
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dibromo-2-hydroxyphenyl)- (9CI)
(CA INDEX NAME)



RN 243135-70-8 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)-, (3S)- (9CI) (CA INDEX NAME)

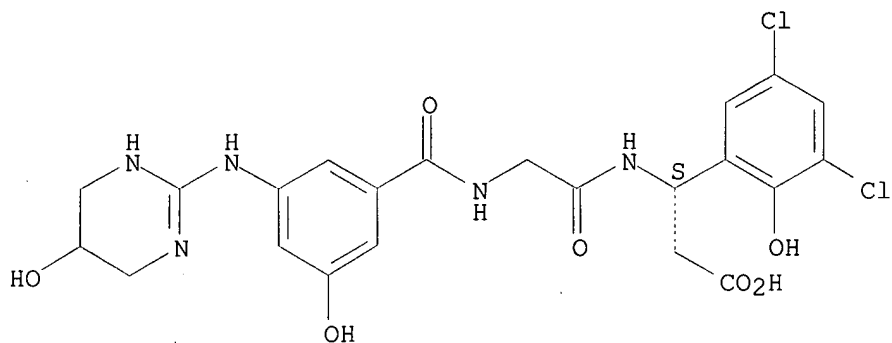
Absolute stereochemistry.



RN 243135-71-9 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, monohydrochloride, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

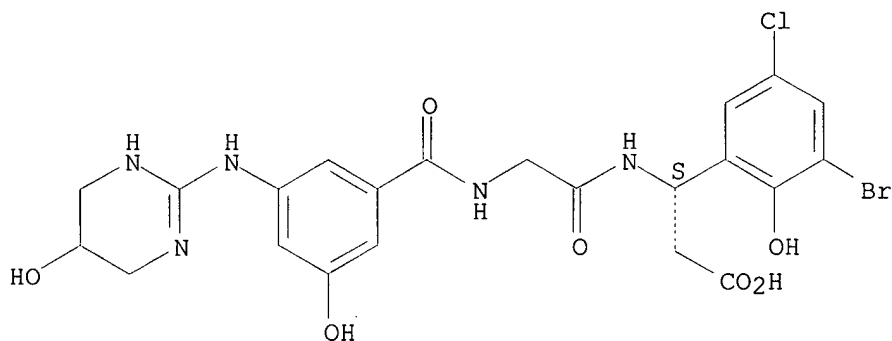


● HCl

RN 243135-72-0 CAPLUS

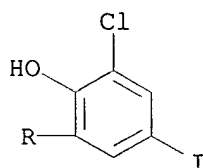
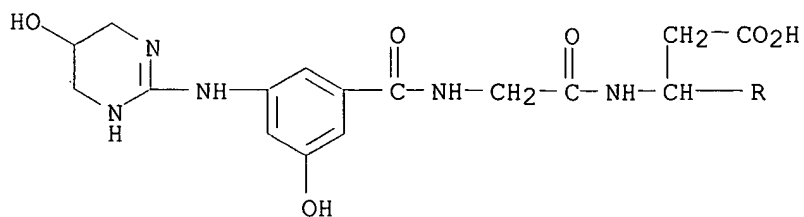
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

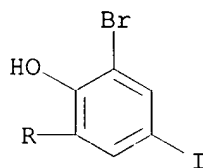
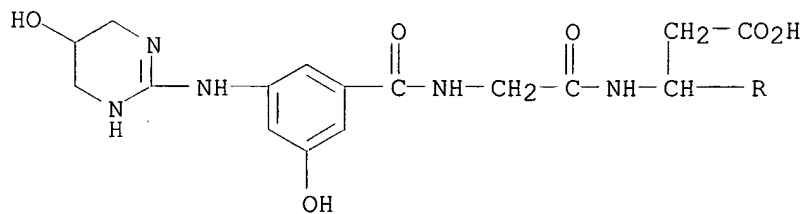


RN 243135-74-2 CAPLUS

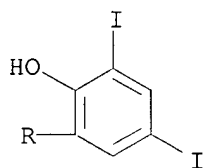
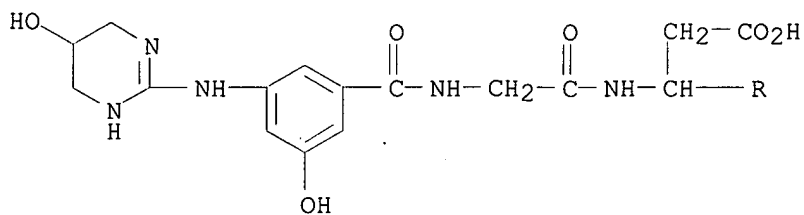
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-chloro-5-iodo-2-hydroxyphenyl)- (9CI) (CA INDEX NAME)



RN 243135-75-3 CAPLUS
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-iodo-2-hydroxyphenyl)- (9CI)
(CA INDEX NAME)



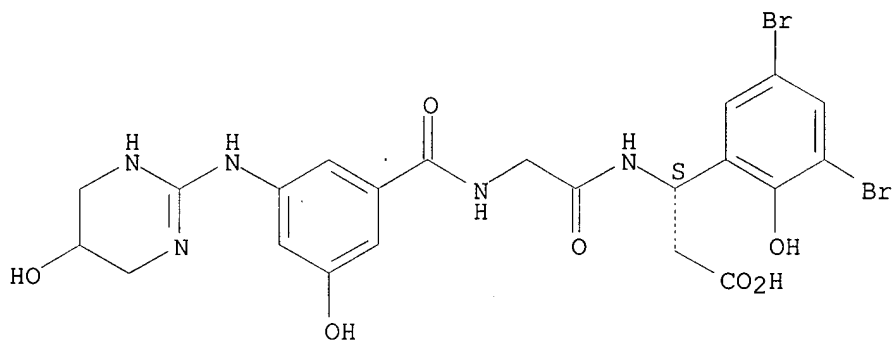
RN 243135-76-4 CAPLUS
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-diiodo-2-hydroxyphenyl)- (9CI)
(CA INDEX NAME)



RN 243135-78-6 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dibromo-2-hydroxyphenyl)-, (3S)-(9CI) (CA INDEX NAME)

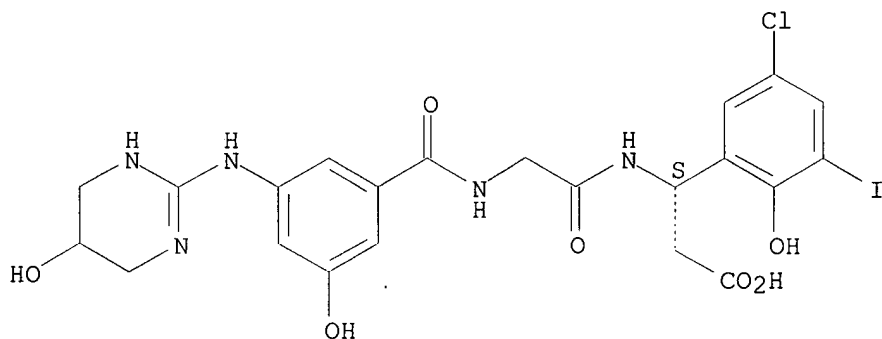
Absolute stereochemistry.



RN 243135-79-7 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-chloro-3-iodo-2-hydroxyphenyl)-, (3S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

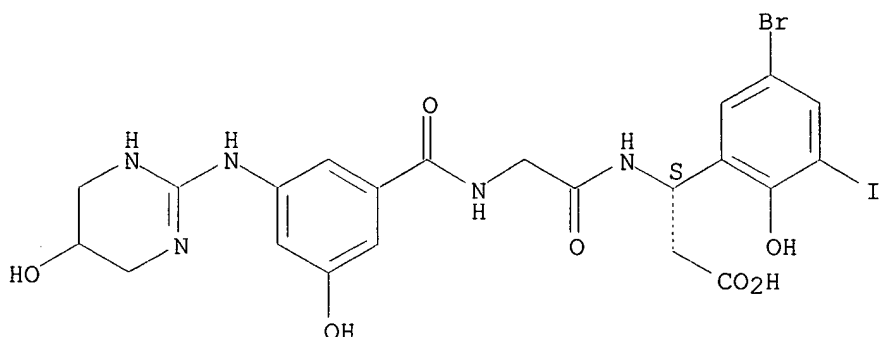


RN 243135-80-0 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-

pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-2-hydroxy-3-iodophenyl)-,
(3S)- (9CI) (CA INDEX NAME)

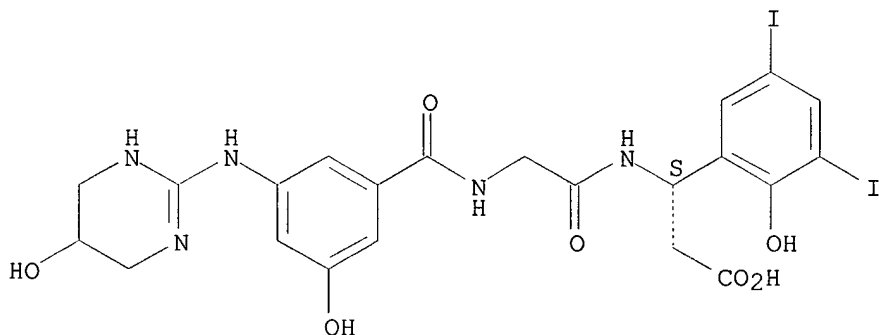
Absolute stereochemistry.



RN 243135-81-1 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-diiodo-2-hydroxyphenyl)-, (3S)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



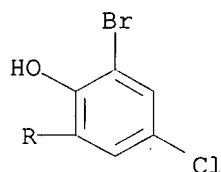
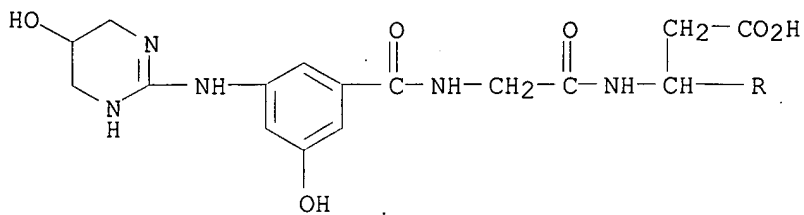
RN 290826-47-0 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, compd. with trifluoromethanol (9CI) (CA INDEX NAME)

CM 1

CRN 243135-63-9

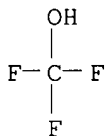
CMF C22 H23 Br Cl N5 O7



CM 2

CRN 1493-11-4

CMF C H F3 O



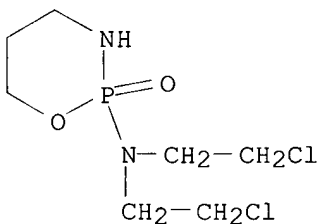
IT 50-18-0, Cyclophosphamide 51-21-8, 5-
 Fluorouracil 15663-27-1, Cisplatin
 23214-92-8, Doxorubicin 33069-62-4,
 Taxol

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
 (Biological study); USES (Uses)

(prepn. of peptidyl integrin antagonists for use in **combination**
 with a chemotherapeutic agent for treatment of neoplasia)

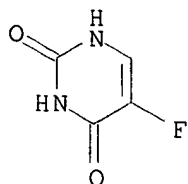
RN 50-18-0 CAPLUS

CN 2H-1,3,2-Oxazaphosphorin-2-amine, N,N-bis(2-chloroethyl)tetrahydro-,
 2-oxide (9CI) (CA INDEX NAME)



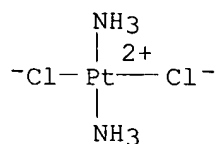
RN 51-21-8 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro- (9CI) (CA INDEX NAME)



RN 15663-27-1 CAPLUS

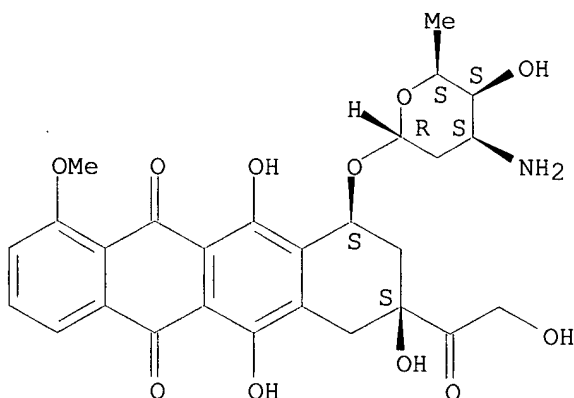
CN Platinum, diamminedichloro-, (SP-4-2)- (9CI) (CA INDEX NAME)



RN 23214-92-8 CAPLUS

CN 5,12-Naphthacenedione, 10-[(3-amino-2,3,6-trideoxy-.alpha.-L-lyxo-hexopyranosyl)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(hydroxyacetyl)-1-methoxy-, (8S,10S)- (9CI) (CA INDEX NAME)

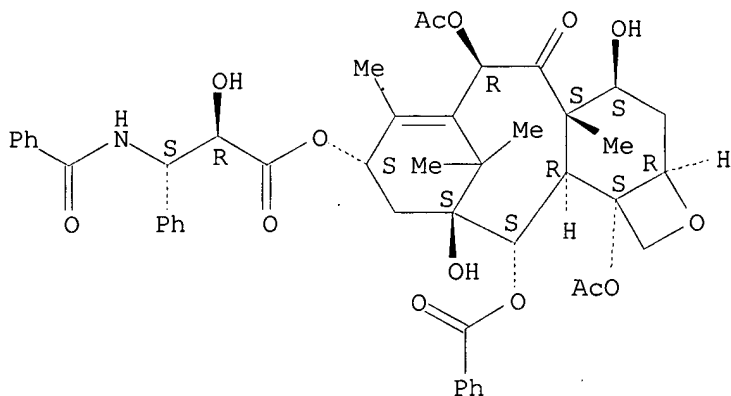
Absolute stereochemistry.



RN 33069-62-4 CAPLUS

CN Benzenepropanoic acid, .beta.-(benzoylamino)-.alpha.-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (.alpha.R,.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



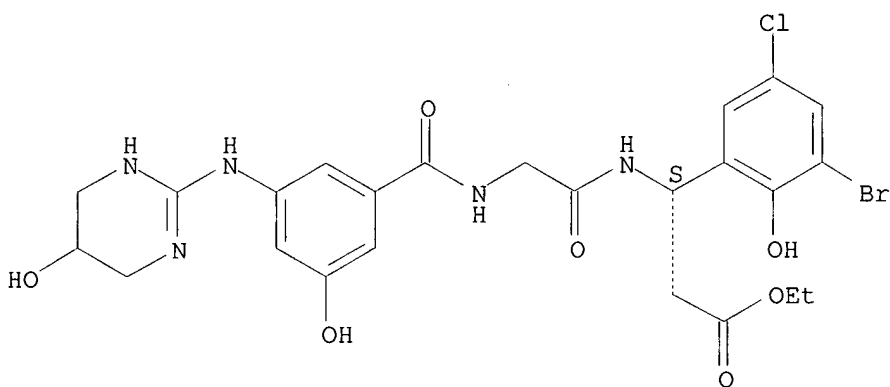
IT **243136-20-1P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, ethyl ester, (3S)- **287485-08-9P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, ethyl ester, (3S)- **290826-70-9P**, .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3S)-, mono(trifluoroacetate) (salt)
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of peptidyl integrin antagonists for use in **combination** with a chemotherapeutic agent for treatment of neoplasia)

RN 243136-20-1 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, ethyl ester, (3S)- (9CI) (CA INDEX NAME)

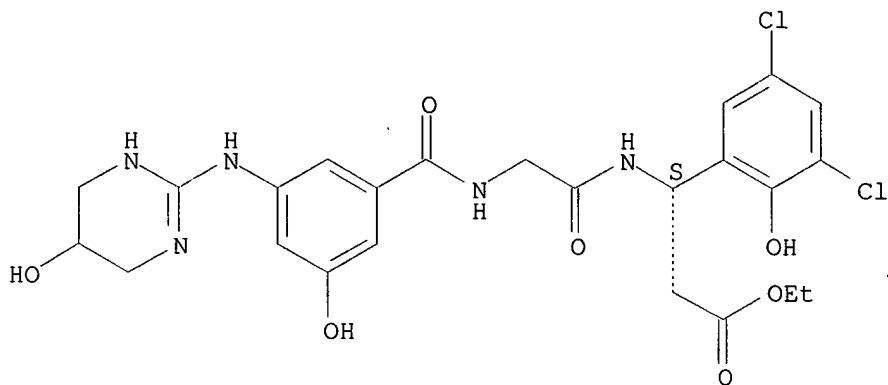
Absolute stereochemistry.



RN 287485-08-9 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, ethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 290826-70-9 CAPLUS

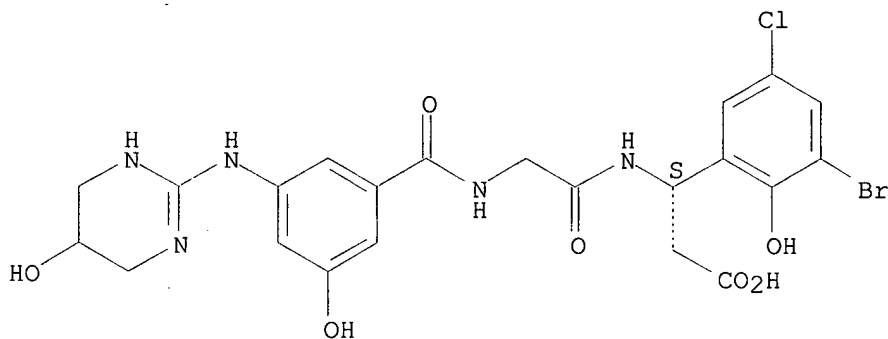
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3S)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 243135-72-0

CMF C22 H23 Br Cl N5 O7

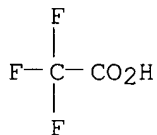
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



REFERENCE COUNT:

9

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L65 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:716096 CAPLUS

DOCUMENT NUMBER: 137:226651

Searched by Barb O'Bryen, STIC 308-4291

TITLE: Combined method for treating hormone-dependent disorders with aromatase inactivator exemestane and other therapeutic agents

INVENTOR(S): Di Salle, Enrico; Piscitelli, Gabriella; Massimini, Giorgio; Purandare, Dinesh; Dekoning, Gans Hendrik

PATENT ASSIGNEE(S): Pharmacia Italia S.p.A., Italy; Pharmacia & Upjohn Company

SOURCE: PCT Int. Appl., 49 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002072106	A2	20020919	WO 2002-EP638	20020118
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.: US 2001-770911 A 20010126

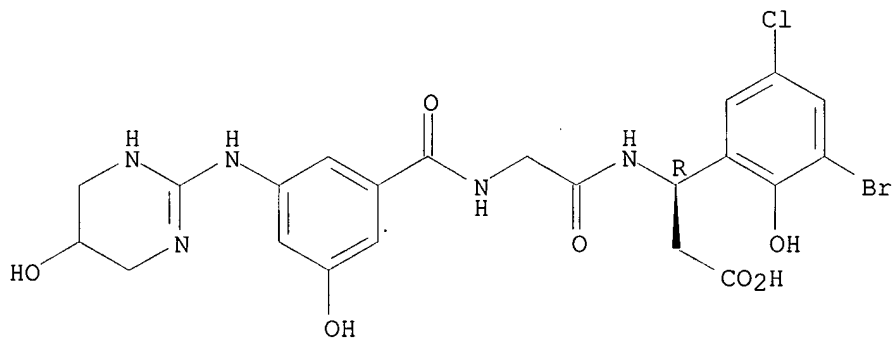
AB A method of preventing and treating estrogen dependent disorders selected from endometriosis, uterine fibroids, dysfunctional uterine bleeding, endometrial hyperplasia, polycystic ovarian disease, fibrocystic breast disease and fibrocystic mastopathy, is disclosed which is comprised of administering to a mammalian patient in need of such treatment an effective amt. of aromatase inactivator exemestane, alone or in combination with addnl. therapeutic agents.

IT 280105-17-1
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(combined method for treating hormone-dependent disorders with aromatase inactivator exemestane and other therapeutic agents)

RN 280105-17-1 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3R)- (9CI) (CA INDEX NAME)

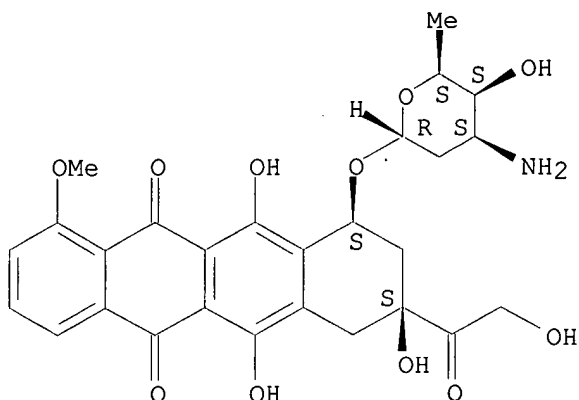
Absolute stereochemistry.



ACCESSION NUMBER: 2002:184907 CAPLUS
DOCUMENT NUMBER: 136:241643
TITLE: Exemestane as chemopreventing agent
INVENTOR(S): Di Salle, Enrico; Piscitelli, Gabriella; Massimini, Giorgio; Purandare, Dinesh; Martini, Alessandro; Muggetti, Lorena
PATENT ASSIGNEE(S): Pharmacia & Upjohn S.p.A., Italy; Pharmacia & Upjohn Company
SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002020020	A1	20020314	WO 2001-EP10172	20010831
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2001089865	A5	20020322	AU 2001-89865	20010831
PRIORITY APPLN. INFO.:			US 2000-658052 A	20000908
			WO 2001-EP10172 W	20010831
AB	The present invention concerns the use of aromatase inhibitor exemestane, either alone or in combination with other therapeutic agents, in the chemoprevention of estrogen dependent cancer in mammals, including humans, at increased risk of the disease. Exemestane treatment (4, 20 or 100 mg/kg/wk, IM), started 1 wk after dimethylbenzanthracene (DMBA) exposure (20 mg/rat, PO) and continued for 19 wk, significantly decreased tumor incidence from 85 % in vehicle treated rats to 13.6 % in the 100 mg/kg treated group. Moreover, exemestane at 100 mg/kg reduced significantly the tumor multiplicity, being 2.55 the no. of tumors/rat in the control groups vs. 0.27 in the treated group. No signs of toxicity were obsd.			
IT	23214-92-8, Doxorubicin 33069-62-4, Paclitaxel 280105-17-1 , SD 7784 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (in combination ; exemestane as chemopreventing agent for estrogen-dependent cancer)			
RN	23214-92-8 CAPLUS			
CN	5,12-Naphthacenedione, 10-[(3-amino-2,3,6-trideoxy-.alpha.-L-lyxo-hexopyranosyl)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(hydroxyacetyl)-1-methoxy-, (8S,10S)- (9CI) (CA INDEX NAME)			

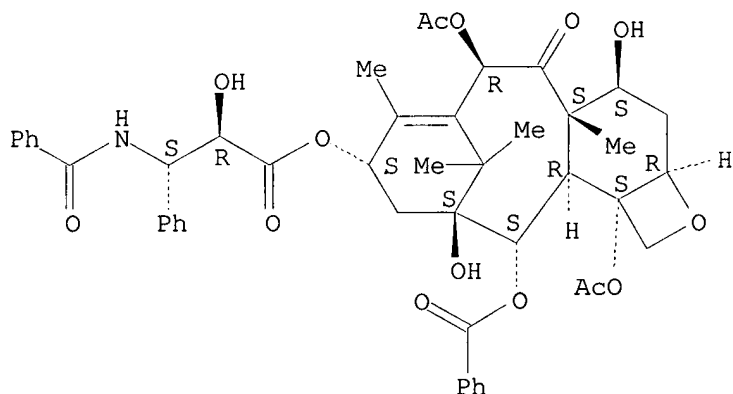
Absolute stereochemistry.



RN 33069-62-4 CAPLUS

CN Benzenepropanoic acid, .beta.-(benzoylamino)-.alpha.-hydroxy-,
(2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-
2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-
tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl
ester, (.alpha.R,.beta.S)- (9CI) (CA INDEX NAME)

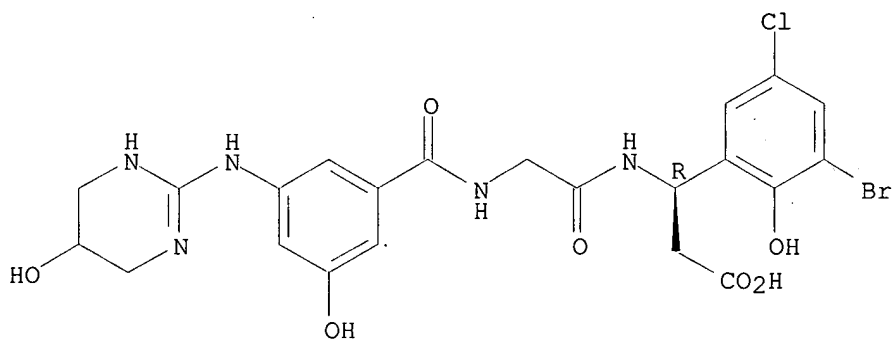
Absolute stereochemistry. Rotation (-).



RN 280105-17-1 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-
pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-,
(3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



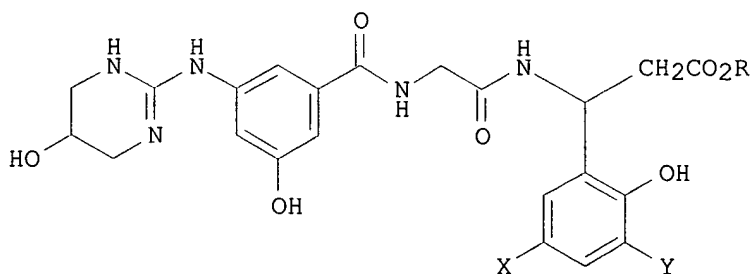
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L65 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:628046 CAPLUS
DOCUMENT NUMBER: 133:223050
TITLE: Preparation of peptidyl integrin antagonists for use in **combination** with a chemotherapeutic agent for treatment of neoplasia
INVENTOR(S): Cunningham, Jay; Gordon, Gary B.; Nickols, G. Allen; Westlin, William F.; Rogers, Thomas E.; Ruminski, Peter G.
PATENT ASSIGNEE(S): G.D. Searle & Co., USA
SOURCE: PCT Int. Appl., 120 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000051686	A1	20000908	WO 2000-US3705	20000301
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6372719	B1	20020416	US 1999-262725	19990304
EP 1161280	A1	20011212	EP 2000-914580	20000301
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JP 2002538177	T2	20021112	JP 2000-602347	20000301
PRIORITY APPLN. INFO.:				
			US 1999-262725	A 19990304
			US 1998-34270	B2 19980304
			WO 2000-US3705	W 20000301
OTHER SOURCE(S): MARPAT 133:223050				
GI				

C₂₂H₂₃BrClN₅O₇

Stereo: ns



AB Peptides I (R = H, alkyl; X, Y = halo) were prep'd. as .alpha.v.beta.3

integrin antagonists which in combination with a chemotherapeutic agent (**cisplatin, cyclophosphamide, 5-fluorouracil, doxorubicin and taxol**) are used for treatment of neoplasia. Thus, 3-bromo-5-chloro-2-hydroxy-.beta.-[[2-[[[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxypyrimidin-2-yl)amino]phenyl]carbonyl]amino]acetyl]amino]benzenepropanoic acid trifluoroacetate was prepd. by peptide coupling of N-glycyl-.beta.-(3-bromo-5-chloro-2-hydroxyphenyl)-.beta.-aminopropionic acid Et ester with 3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxypyrimidin-2-yl)amino]benzoic acid. Peptides I delayed the growth of tumors in mice, particularly when combined with a chemotherapeutic agent.

IT 50-18-0P, Cyclophosphamide 51-21-8P, 5-

Fluorouracil 15663-27-1P, Cisplatin

23214-92-8P, Doxorubicin 33069-62-4P,

Taxol 243135-63-9P 243135-65-1P

243135-66-2P 243135-67-3P 243135-68-4P

243135-69-5P 243135-70-8P 243135-71-9P

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243135-76-4P 243135-78-6P 243135-79-7P

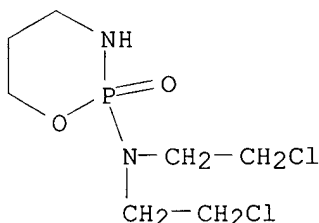
243135-80-0P 243135-81-1P 290826-47-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptidyl integrin antagonists for use in **combination** with a chemotherapeutic agent for treatment of neoplasia)

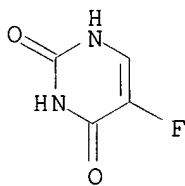
RN 50-18-0 CAPLUS

CN 2H-1,3,2-Oxazaphosphorin-2-amine, N,N-bis(2-chloroethyl)tetrahydro-, 2-oxide (9CI) (CA INDEX NAME)



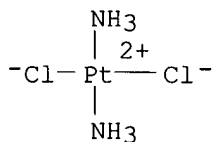
RN 51-21-8 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro- (9CI) (CA INDEX NAME)



RN 15663-27-1 CAPLUS

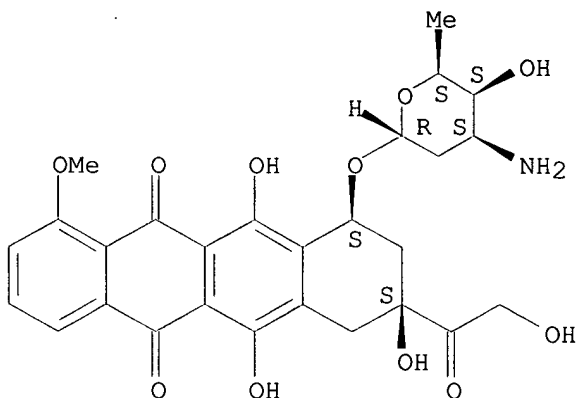
CN Platinum, diamminedichloro-, (SP-4-2)- (9CI) (CA INDEX NAME)



RN 23214-92-8 CAPLUS

CN 5,12-Naphthacenedione, 10-[(3-amino-2,3,6-trideoxy-.alpha.-L-lyxo-hexopyranosyl)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(hydroxyacetyl)-1-methoxy-, (8S,10S)- (9CI) (CA INDEX NAME)

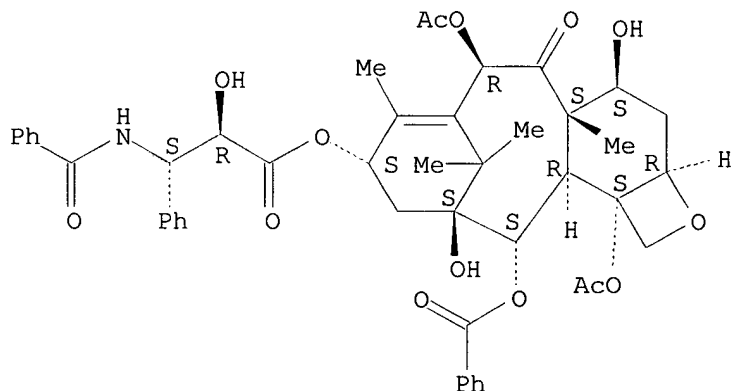
Absolute stereochemistry.



RN 33069-62-4 CAPLUS

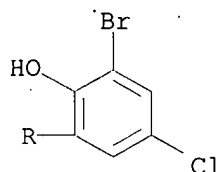
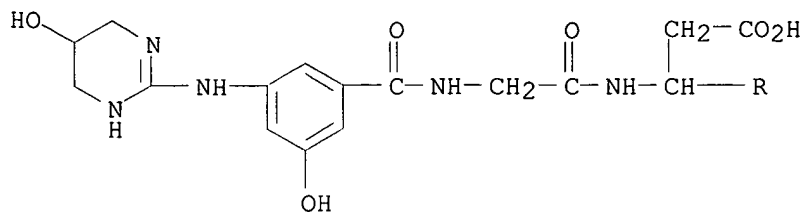
CN Benzenepropanoic acid, .beta.-(benzoylamino)-.alpha.-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (.alpha.R,.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

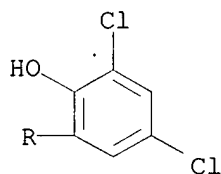
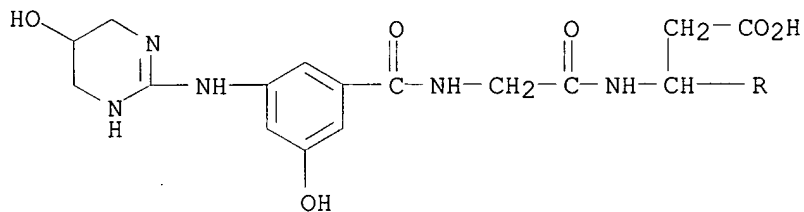


RN 243135-63-9 CAPLUS

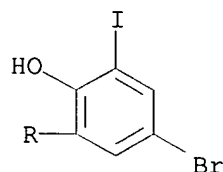
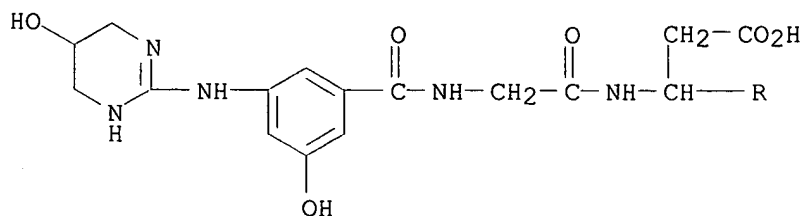
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)- (9CI) (CA INDEX NAME)



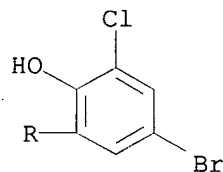
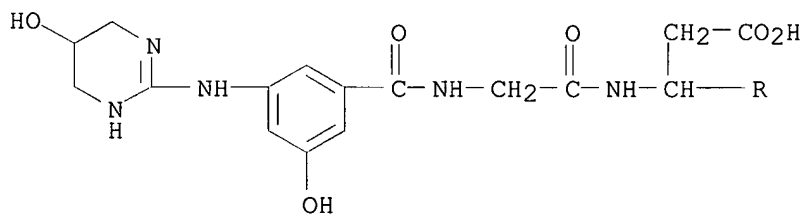
RN 243135-65-1 CAPLUS
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)- (9CI)
(CA INDEX NAME)



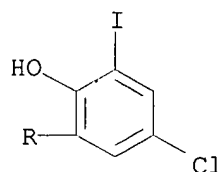
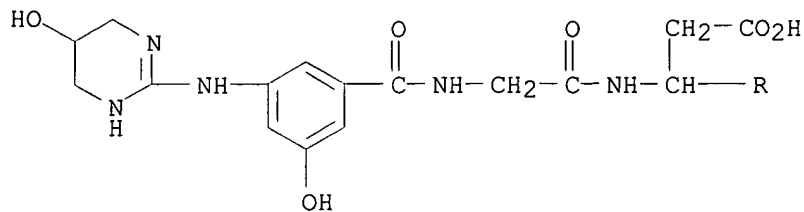
RN 243135-66-2 CAPLUS
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-iodo-2-hydroxyphenyl)- (9CI)
(CA INDEX NAME)



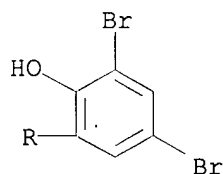
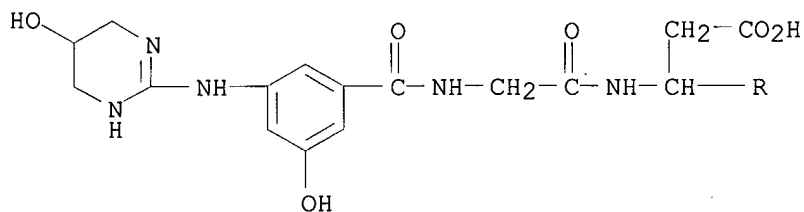
RN 243135-67-3 CAPLUS
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)-
(9CI) (CA INDEX NAME)



RN 243135-68-4 CAPLUS
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-chloro-3-iodo-2-hydroxyphenyl)-
(9CI) (CA INDEX NAME)

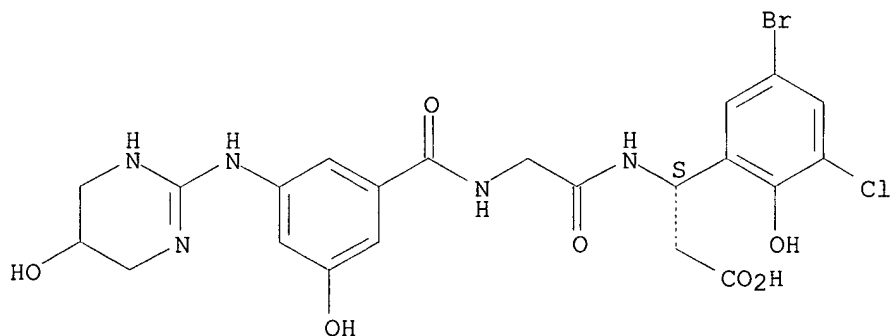


RN 243135-69-5 CAPLUS
 CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dibromo-2-hydroxyphenyl)- (9CI)
 (CA INDEX NAME)



RN 243135-70-8 CAPLUS
 CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)-, (3S)- (9CI) (CA INDEX NAME)

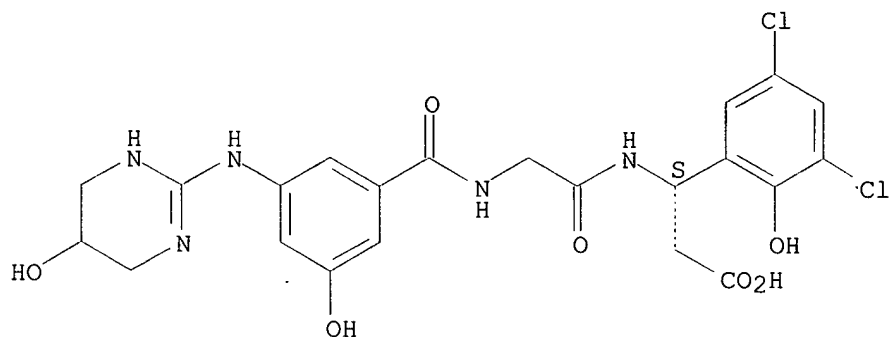
Absolute stereochemistry.



RN 243135-71-9 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, monohydrochloride, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

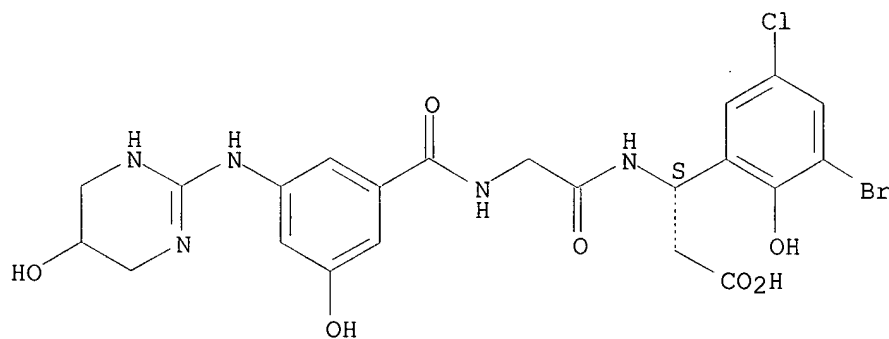


● HCl

RN 243135-72-0 CAPLUS

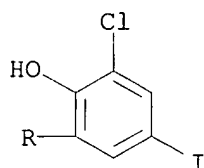
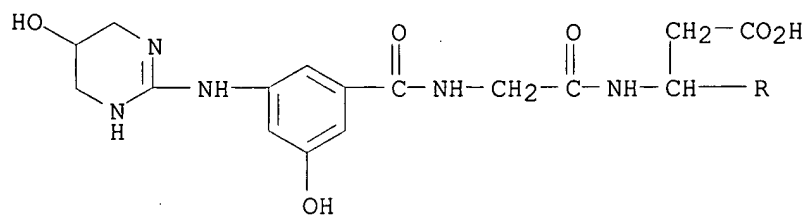
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

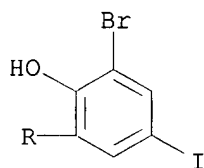
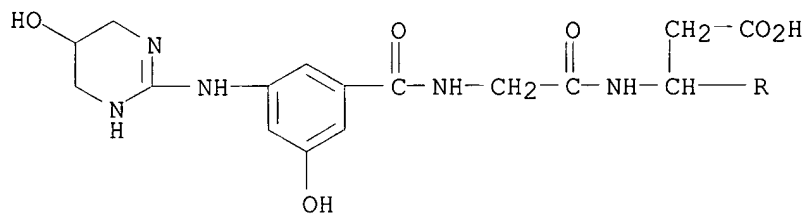


RN 243135-74-2 CAPLUS

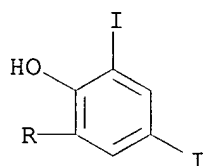
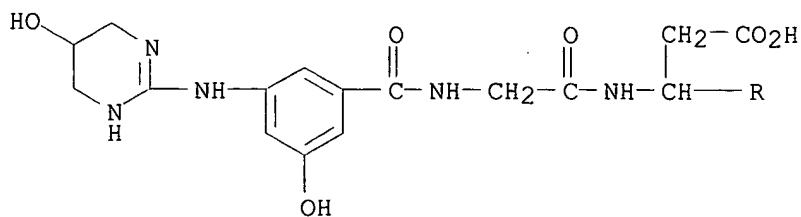
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-chloro-5-iodo-2-hydroxyphenyl)-, (9CI) (CA INDEX NAME)



RN 243135-75-3 CAPLUS
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-iodo-2-hydroxyphenyl)- (9CI)
(CA INDEX NAME)



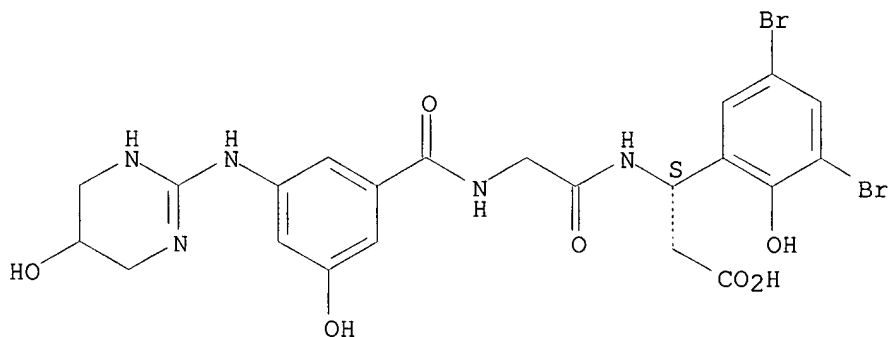
RN 243135-76-4 CAPLUS
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-diiodo-2-hydroxyphenyl)- (9CI)
(CA INDEX NAME)



RN 243135-78-6 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dibromo-2-hydroxyphenyl)-, (3S)-(9CI) (CA INDEX NAME)

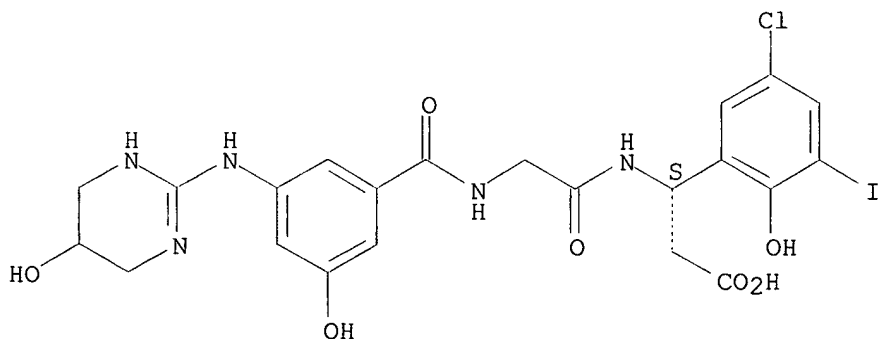
Absolute stereochemistry.



RN 243135-79-7 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-chloro-3-iodo-2-hydroxyphenyl)-, (3S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

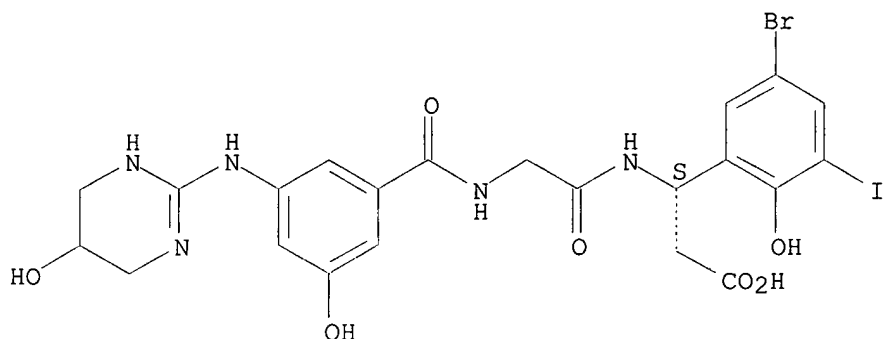


RN 243135-80-0 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-

pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-2-hydroxy-3-iodophenyl)-,
(3S)- (9CI) (CA INDEX NAME)

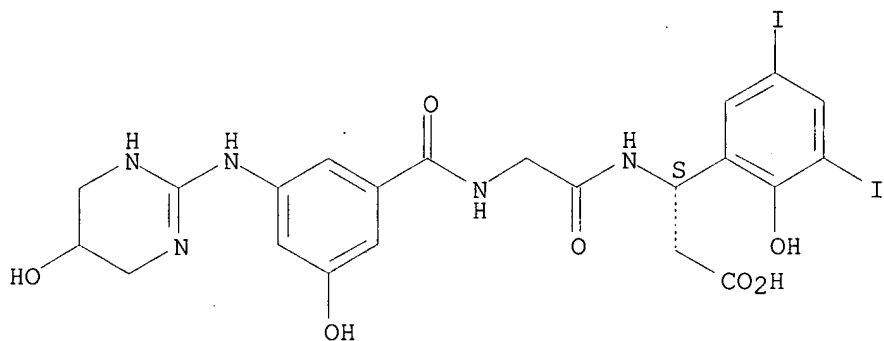
Absolute stereochemistry.



RN 243135-81-1 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-diiodo-2-hydroxyphenyl)-, (3S)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



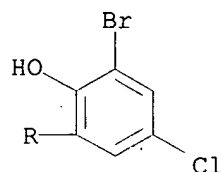
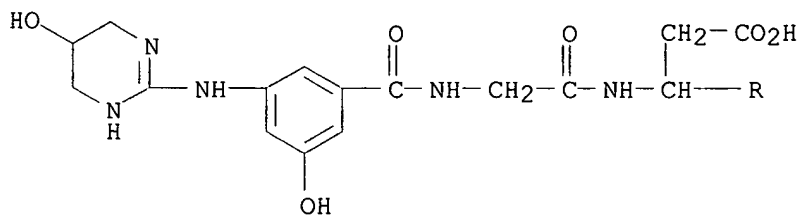
RN 290826-47-0 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, compd. with trifluoromethanol (9CI) (CA INDEX NAME)

CM 1

CRN 243135-63-9

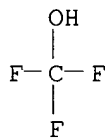
CMF C22 H23 Br Cl N5 O7



CM 2

CRN 1493-11-4

CMF C H F3 O



IT 243136-20-1P 287485-08-9P 290826-70-9P

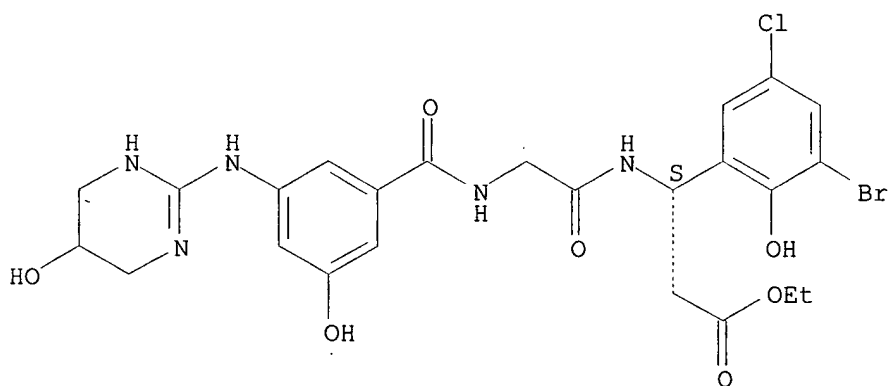
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of peptidyl integrin antagonists for use in **combination** with a chemotherapeutic agent for treatment of neoplasia)

RN 243136-20-1 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, ethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

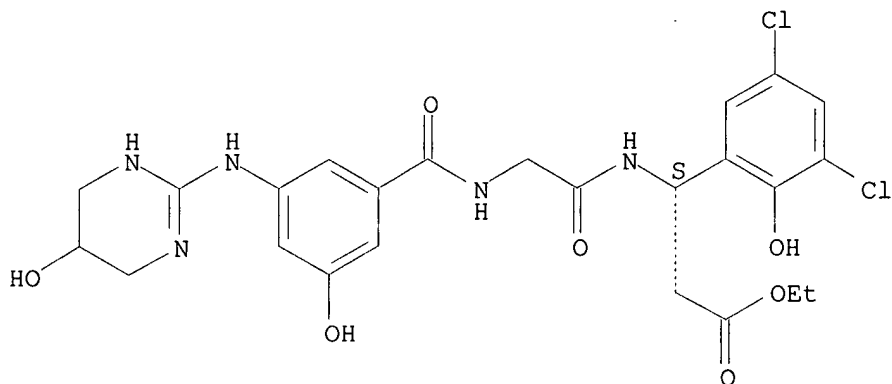


RN 287485-08-9 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-

pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, ethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

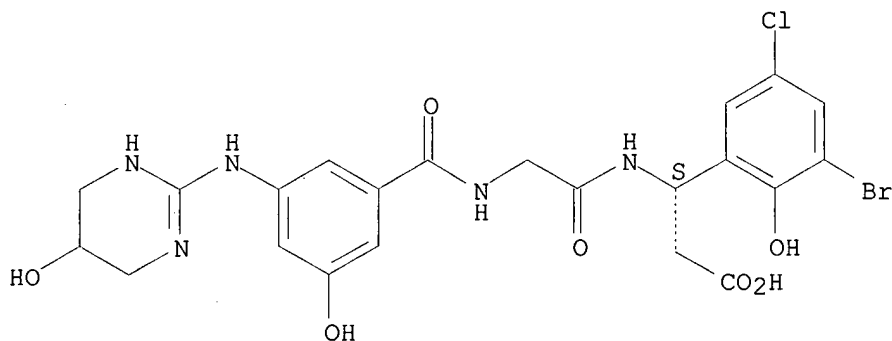


RN 290826-70-9 CAPLUS
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3S)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

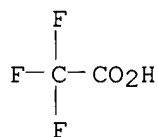
CRN 243135-72-0
CMF C22 H23 Br Cl N5 O7

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L65 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:456950 CAPLUS

DOCUMENT NUMBER: 133:84244

TITLE: Method of using a cyclooxygenase-2 inhibitor and an integrin antagonist as a **combination** therapy in the treatment of neoplasia

INVENTOR(S): McKearn, John P.; Gordon, Gary; Cunningham, James J.; Gately, Stephen T.; Koki, Alane T.; Masferrer, Jaime L.

PATENT ASSIGNEE(S): G.D. Searle & Co., USA

SOURCE: PCT Int. Appl., 348 pp.

CODEN: PIXXD2

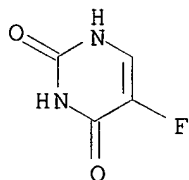
DOCUMENT TYPE: Patent

LANGUAGE: English

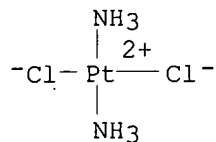
FAMILY ACC. NUM. COUNT: 11

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000038786	A2	20000706	WO 1999-US30692	19991222
WO 2000038786	A3	20010308		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2356302	AA	20000706	CA 1999-2356302	19991222
EP 1140179	A2	20011010	EP 1999-966594	19991222
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002533422	T2	20021008	JP 2000-590734	19991222
PRIORITY APPLN. INFO.: US 1998-113786P P 19981223				
WO 1999-US30692 W 19991222				
AB Methods are provided to treat or prevent neoplasia disorders in a mammal using a combination of a cyclooxygenase-2 inhibitor, an integrin antagonist and an antineoplastic agent.				
IT 51-21-8, 5-Fluorouracil 15663-27-1, Cisplatin 23214-92-8, Doxorubicin 33069-62-4, Paclitaxel 280105-13-7 280105-14-8 280105-17-1 280105-18-2 280105-19-3				
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)				
(cyclooxygenase-2 inhibitor and integrin antagonist in combination for neoplasia treatment)				
RN 51-21-8 CAPLUS				
CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro- (9CI) (CA INDEX NAME)				

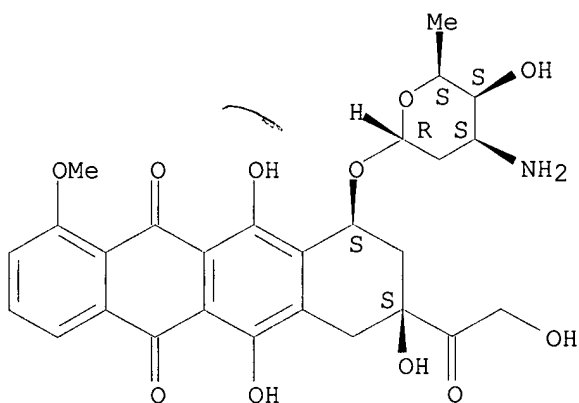


RN 15663-27-1 CAPLUS
 CN Platinum, diamminedichloro-, (SP-4-2)- (9CI) (CA INDEX NAME)



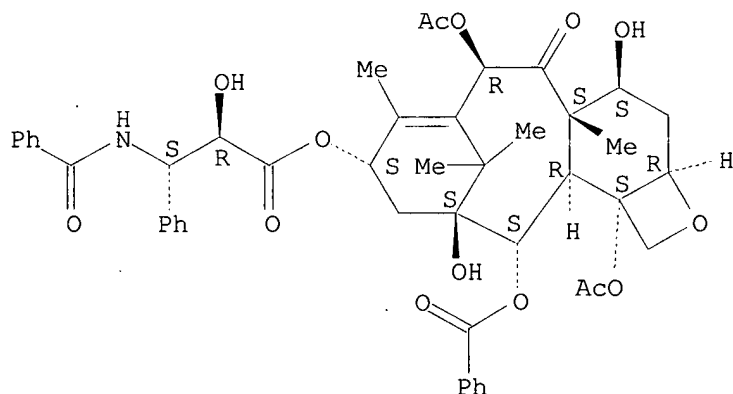
RN 23214-92-8 CAPLUS
 CN 5,12-Naphthacenedione, 10-[(3-amino-2,3,6-trideoxy-.alpha.-L-lyxo-hexopyranosyl)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(hydroxyacetyl)-1-methoxy-, (8S,10S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



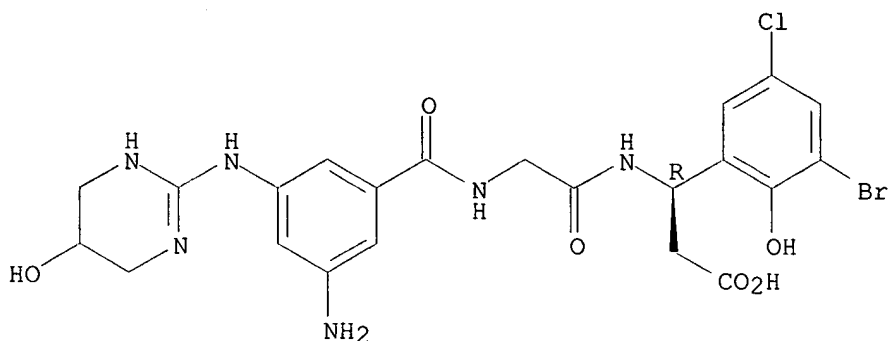
RN 33069-62-4 CAPLUS
 CN Benzenepropanoic acid, .beta.-(benzoylamino)-.alpha.-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (.alpha.R,.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



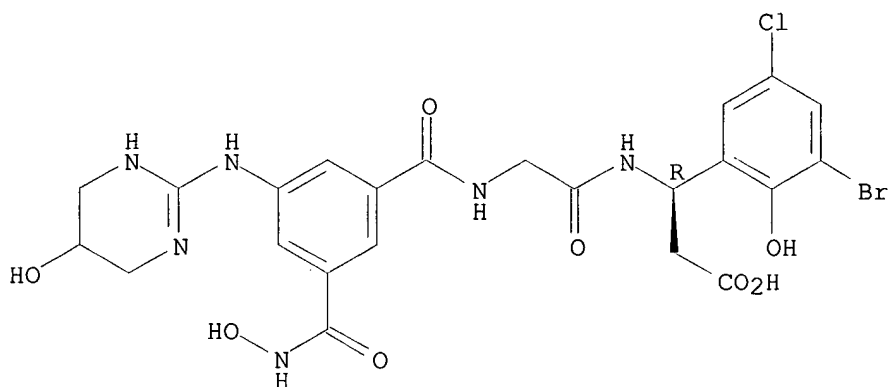
RN 280105-13-7 CAPLUS
 CN .beta.-Alanine, N-[3-amino-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



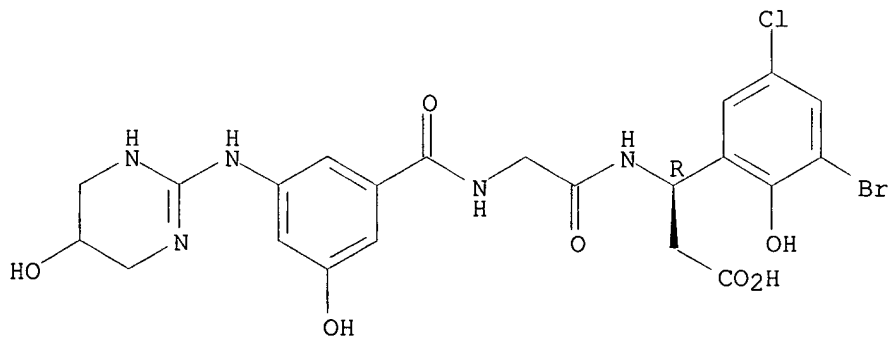
RN 280105-14-8 CAPLUS
 CN .beta.-Alanine, N-[3-[(hydroxyamino)carbonyl]-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 280105-17-1 CAPLUS
 CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3R)- (9CI) (CA INDEX NAME)

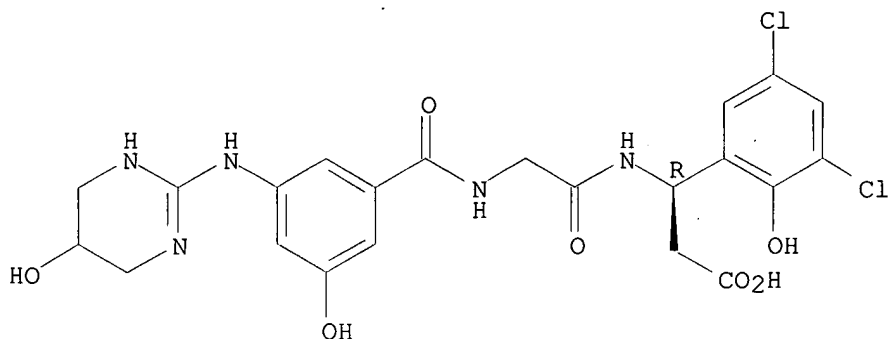
Absolute stereochemistry.



RN 280105-18-2 CAPLUS
 CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-

pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, (3R)-
(9CI) (CA INDEX NAME)

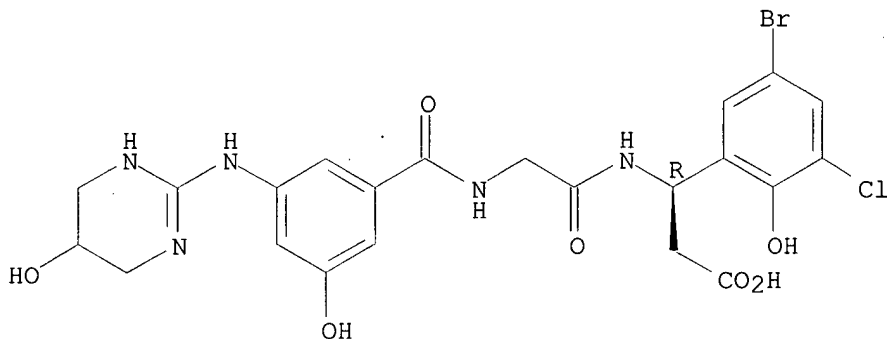
Absolute stereochemistry.



RN 280105-19-3 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L65 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:456916 CAPLUS

DOCUMENT NUMBER: 133:68929

TITLE: Use of a matrix metalloproteinase inhibitor and an integrin antagonist in the treatment of neoplasia

INVENTOR(S): McKearn, John P.; Gordon, Gary; Cunningham, James J.; Gately, Stephen T.; Koki, Alane T.; Masferrer, Jaime L.

PATENT ASSIGNEE(S): G. D. Searle & Co., USA

SOURCE: PCT Int. Appl., 358 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 11

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000038719	A1	20000706	WO 1999-US30700	19991222
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,				

Searched by Barb O'Bryen, STIC 308-4291

MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2356402 AA 20000706 CA 1999-2356402 19991222

EP 1140183 A1 20011010 EP 1999-968942 19991222

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO

JP 2002533407 T2 20021008 JP 2000-590670 19991222

PRIORITY APPLN. INFO.:

US 1998-113786P P 19981223

WO 1999-US30700 W 19991222

AB Methods are provided to treat or prevent neoplasia disorders in a mammal using a combination of a matrix metalloproteinase inhibitor, an integrin antagonist, and an antineoplastic agent.

IT 50-18-0, Cyclophosphamide 51-21-8, 5-

Fluorouracil 15663-27-1, Cisplatin

23214-92-8, Doxorubicin 33069-62-4, Paclitaxel

280105-13-7 280105-14-8 280105-17-1

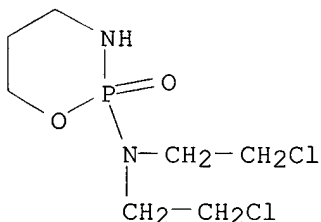
280105-18-2 280105-19-3

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(matrix metalloproteinase inhibitor and integrin antagonist in neoplasia treatment)

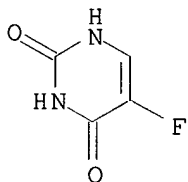
RN 50-18-0 CAPLUS

CN 2H-1,3,2-Oxazaphosphorin-2-amine, N,N-bis(2-chloroethyl)tetrahydro-, 2-oxide (9CI) (CA INDEX NAME)



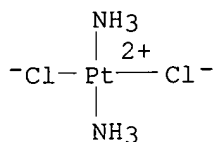
RN 51-21-8 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro- (9CI) (CA INDEX NAME)



RN 15663-27-1 CAPLUS

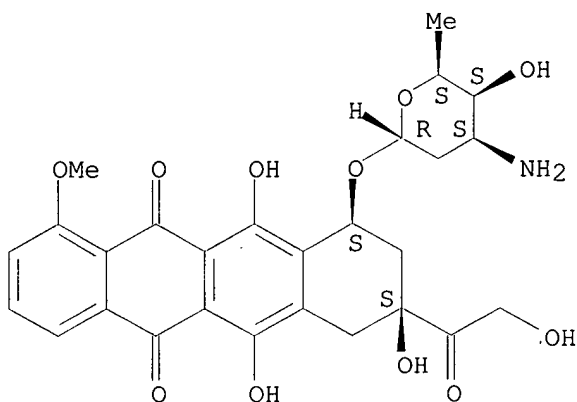
CN Platinum, diamminedichloro-, (SP-4-2)- (9CI) (CA INDEX NAME)



RN 23214-92-8 CAPLUS

CN 5,12-Naphthacenedione, 10-[(3-amino-2,3,6-trideoxy-.alpha.-L-lyxo-hexopyranosyl)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(hydroxyacetyl)-1-methoxy-, (8S,10S)- (9CI) (CA INDEX NAME)

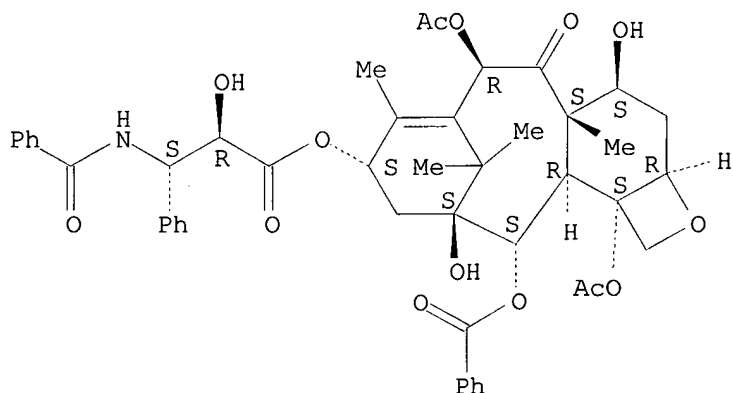
Absolute stereochemistry.



RN 33069-62-4 CAPLUS

CN Benzenepropanoic acid, .beta.-(benzoylamino)-.alpha.-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (.alpha.R,.beta.S)- (9CI) (CA INDEX NAME)

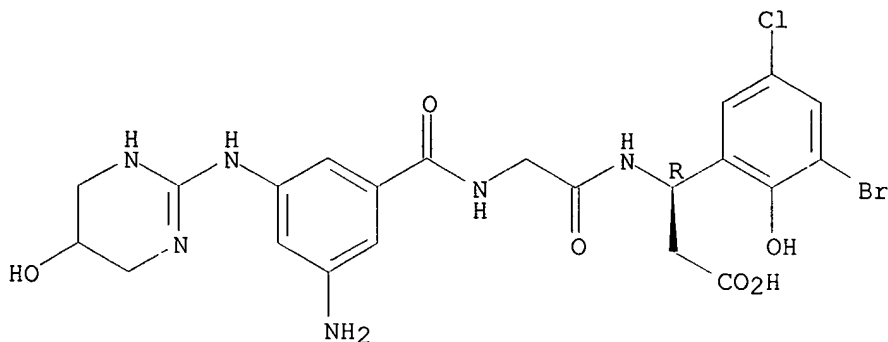
Absolute stereochemistry. Rotation (-).



RN 280105-13-7 CAPLUS

CN .beta.-Alanine, N-[3-amino-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3R)- (9CI) (CA INDEX NAME)

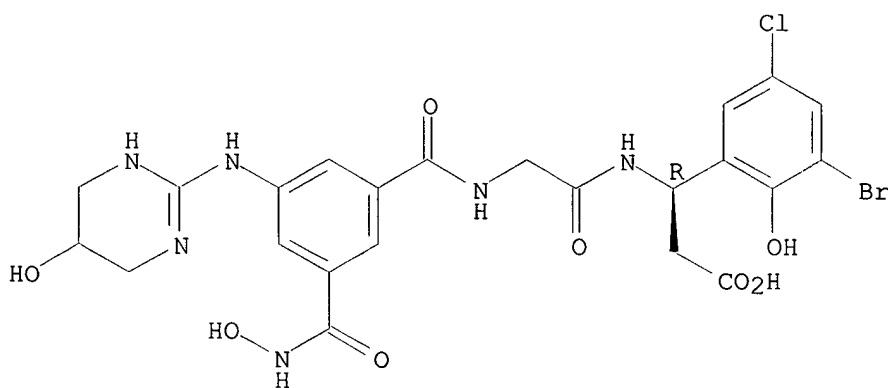
Absolute stereochemistry.



RN 280105-14-8 CAPLUS

CN .beta.-Alanine, N-[3-[(hydroxyamino)carbonyl]-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3R)- (9CI) (CA INDEX NAME)

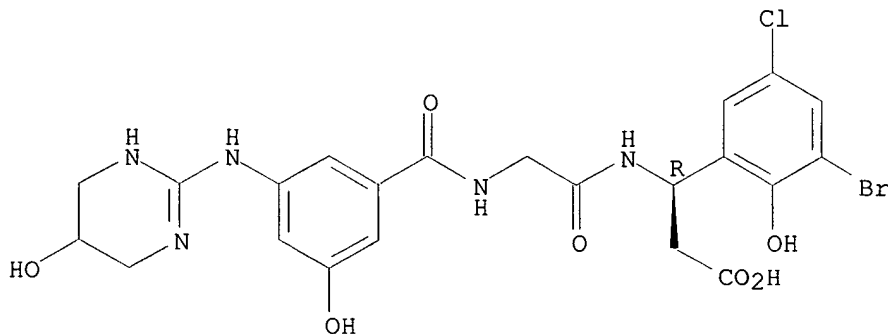
Absolute stereochemistry.



RN 280105-17-1 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3R)- (9CI) (CA INDEX NAME)

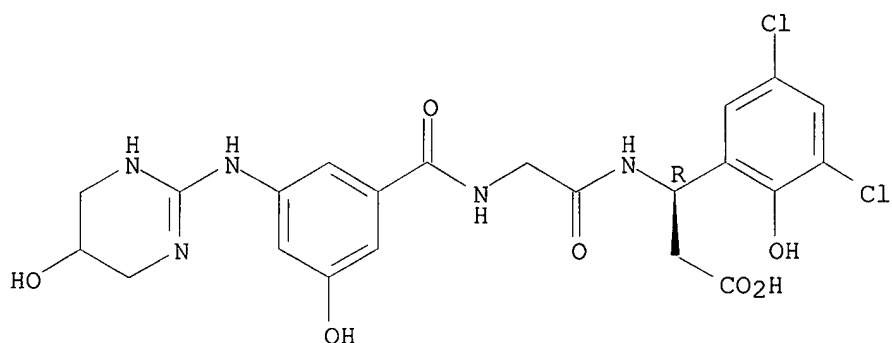
Absolute stereochemistry.



RN 280105-18-2 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, (3R)- (9CI) (CA INDEX NAME)

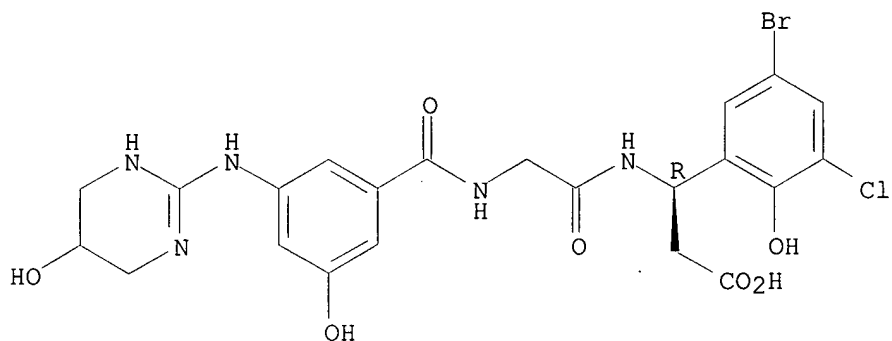
Absolute stereochemistry.



RN 280105-19-3 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L65 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:456912 CAPLUS

DOCUMENT NUMBER: 133:68927

TITLE: Method of using an integrin antagonist and radiation therapy as **combination** therapy in the treatment of neoplasia

INVENTOR(S): McKearn, John P.; Gordon, Gary; Cunningham, James J.; Gately, Stephen T.; Koki, Alane T.; Masferrer, Jaime L.

PATENT ASSIGNEE(S): G.D. Searle and Co., USA

SOURCE: PCT Int. Appl., 95 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 11

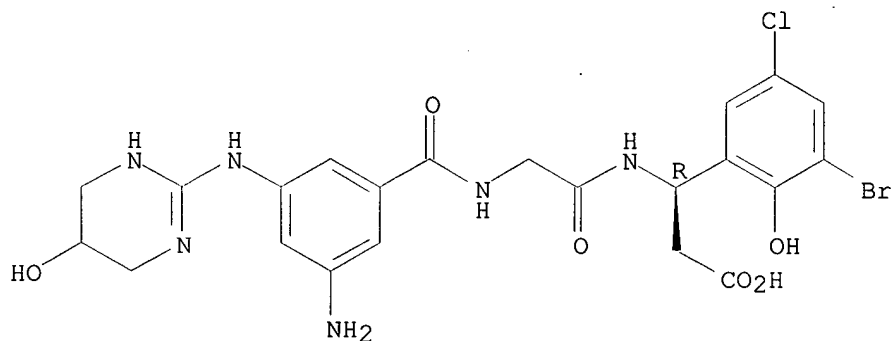
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000038715	A2	20000706	WO 1999-US30621	19991222
WO 2000038715	A3	20010104		

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,

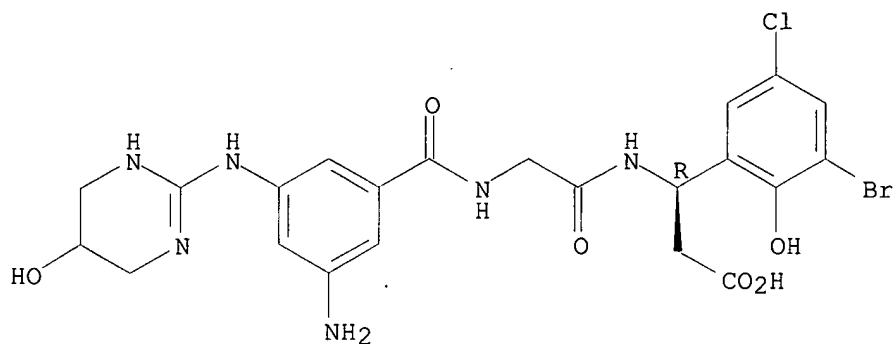
IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
CA 2356748 AA 20000706 CA 1999-2356748 19991222
EP 1140177 A2 20011010 EP 1999-966558 19991222
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO
JP 2002533404 T2 20021008 JP 2000-590666 19991222
PRIORITY APPLN. INFO.: US 1998-113786P P 19981223
WO 1999-US30621 W 19991222
AB Methods are provided to treat neoplasia disorders in a mammal using a
combination of radiation and an integrin antagonist.
IT 280105-13-7 280105-13-7D, derivs. 280105-14-8
280105-14-8D, derivs. 280105-17-1 280105-17-1D
, derivs. 280105-18-2 280105-18-2D, derivs.
280105-19-3 280105-19-3D, derivs.
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
(Uses)
(integrin antagonist and radiation therapy **combination** for
treatment of neoplasia)
RN 280105-13-7 CAPLUS
CN .beta.-Alanine, N-[3-amino-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-
pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-,
(3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 280105-13-7 CAPLUS
CN .beta.-Alanine, N-[3-amino-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-
pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-,
(3R)- (9CI) (CA INDEX NAME)

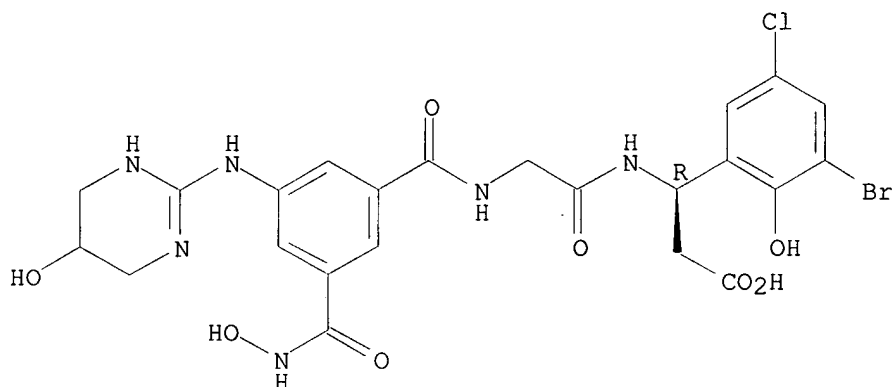
Absolute stereochemistry.



RN 280105-14-8 CAPLUS

CN .beta.-Alanine, N-[3-[(hydroxyamino)carbonyl]-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3R)- (9CI) (CA INDEX NAME)

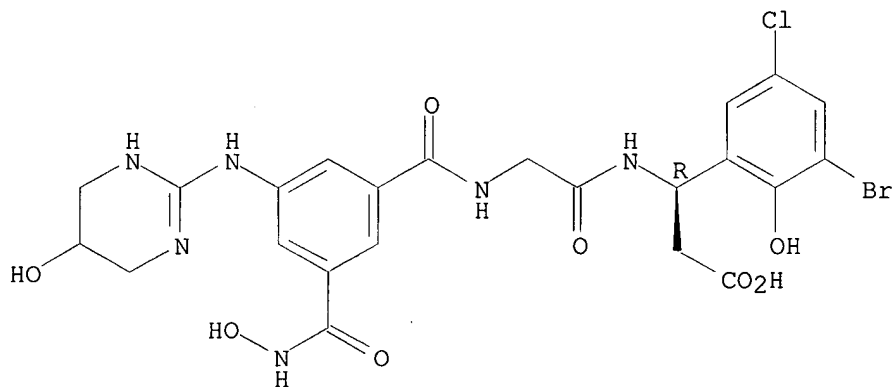
Absolute stereochemistry.



RN 280105-14-8 CAPLUS

CN .beta.-Alanine, N-[3-[(hydroxyamino)carbonyl]-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

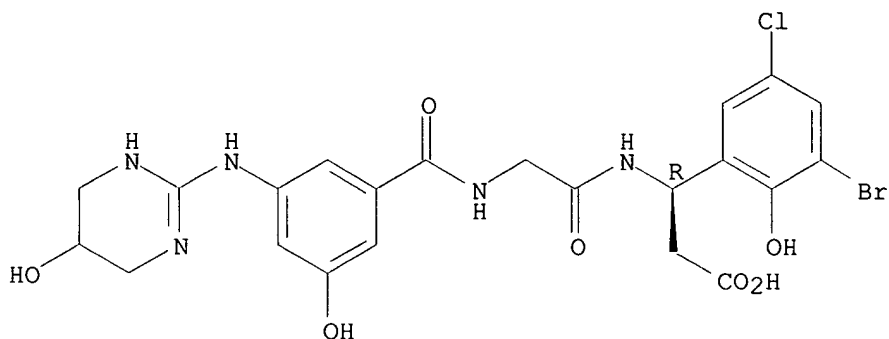


RN 280105-17-1 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-

pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-,
(3R)- (9CI) (CA INDEX NAME)

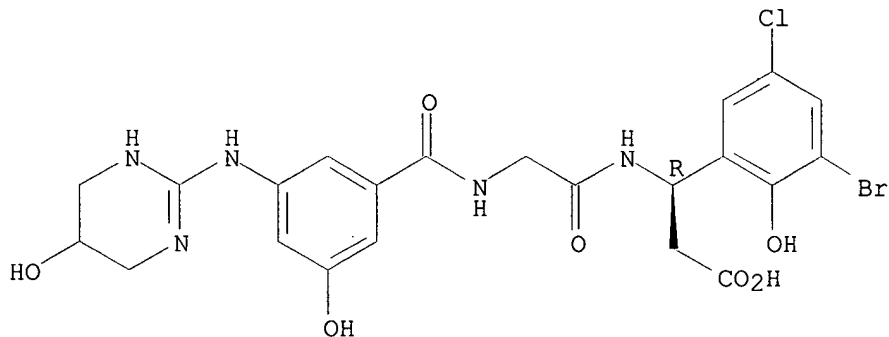
Absolute stereochemistry.



RN 280105-17-1 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-,
(3R)- (9CI) (CA INDEX NAME)

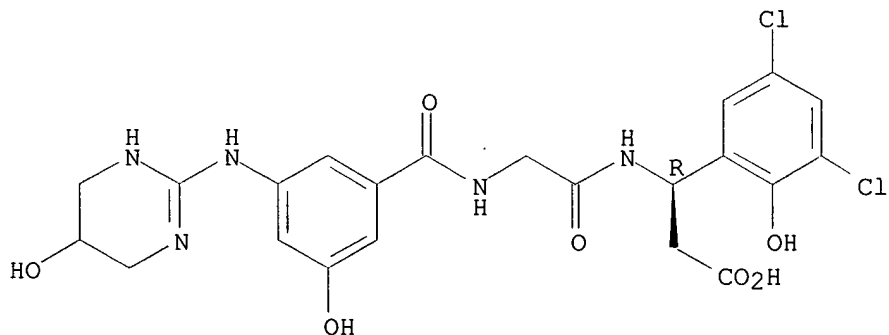
Absolute stereochemistry.



RN 280105-18-2 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, (3R)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

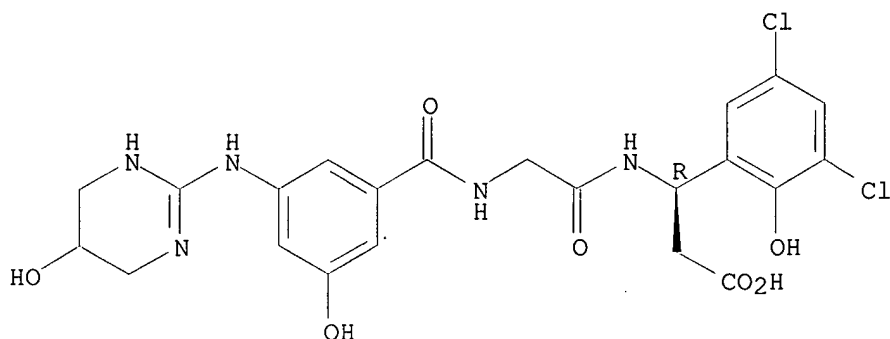


RN 280105-18-2 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-

pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, (3R)-
(9CI) (CA INDEX NAME)

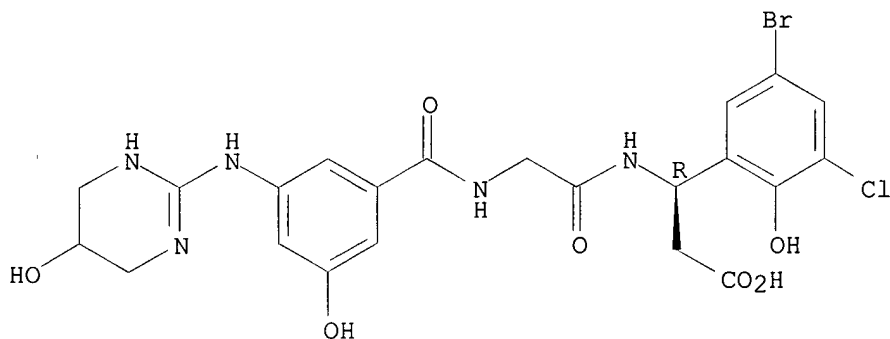
Absolute stereochemistry.



RN 280105-19-3 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)-, (3R)- (9CI) (CA INDEX NAME)

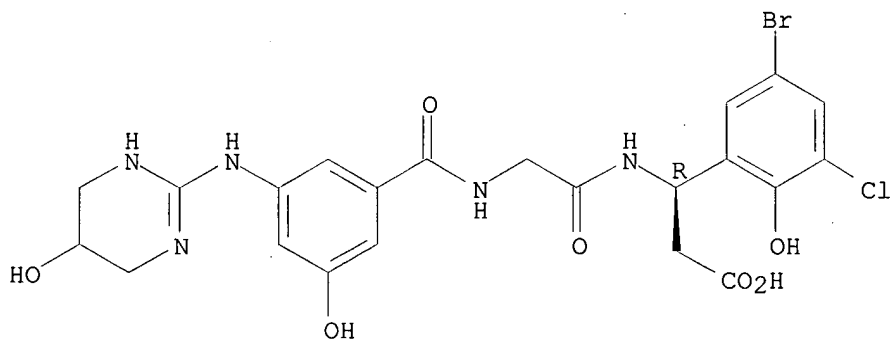
Absolute stereochemistry.



RN 280105-19-3 CAPLUS

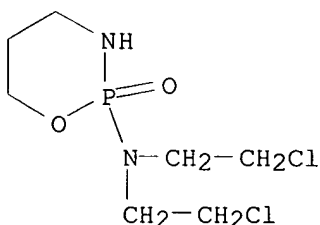
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

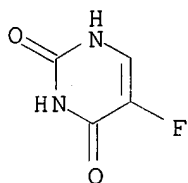


ACCESSION NUMBER: 2000:456866 CAPLUS
DOCUMENT NUMBER: 133:84239
TITLE: Method of using an integrin antagonist and one or more antineoplastic agents as a **combination** therapy in the treatment of neoplasia
INVENTOR(S): McKearn, John P.; Gordon, Gary; Cunningham, James J.; Gately, Stephen T.; Koki, Alane T.; Masferrer, Jaime L.
PATENT ASSIGNEE(S): G. D. Searle & Co., USA
SOURCE: PCT Int. Appl., 220 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 11
PATENT INFORMATION:

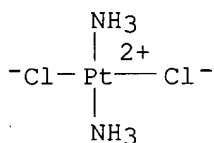
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000038665	A2	20000706	WO 1999-US30670	19991222
WO 2000038665	A3	20001116		
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2356462	AA	20000706	CA 1999-2356462	19991222
EP 1140193	A2	20011010	EP 1999-968529	19991222
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002533387	T2	20021008	JP 2000-590619	19991222
PRIORITY APPLN. INFO.: US 1998-113786P P 19981223				
WO 1999-US30670 W 19991222				
AB	The present invention provides methods to treat or prevent neoplasia disorders in a mammal using a combination of an integrin antagonist and an antineoplastic agent.			
IT	50-18-0, Cyclophosphamide 51-21-8, 5-Fluorouracil 15663-27-1, Cisplatin 23214-92-8, Doxorubicin 33069-62-4, Paclitaxel 280105-13-7 280105-14-8 280105-17-1 280105-18-2 280105-19-3			
RL:	BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (integrin antagonist-antineoplastic agent combination for neoplasia treatment)			
RN	50-18-0 CAPLUS			
CN	2H-1,3,2-Oxazaphosphorin-2-amine, N,N-bis(2-chloroethyl)tetrahydro-, 2-oxide (9CI) (CA INDEX NAME)			



RN 51-21-8 CAPLUS
 CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro- (9CI) (CA INDEX NAME)

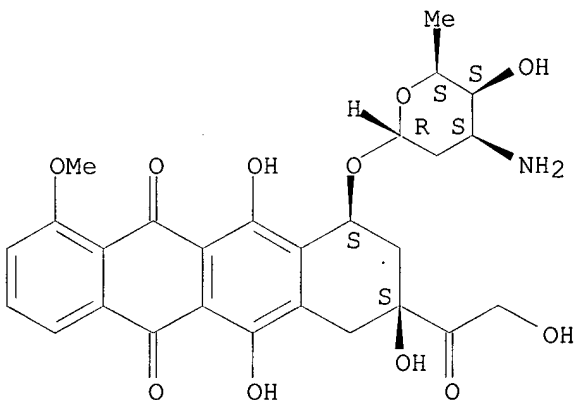


RN 15663-27-1 CAPLUS
 CN Platinum, diamminedichloro-, (SP-4-2)- (9CI) (CA INDEX NAME)



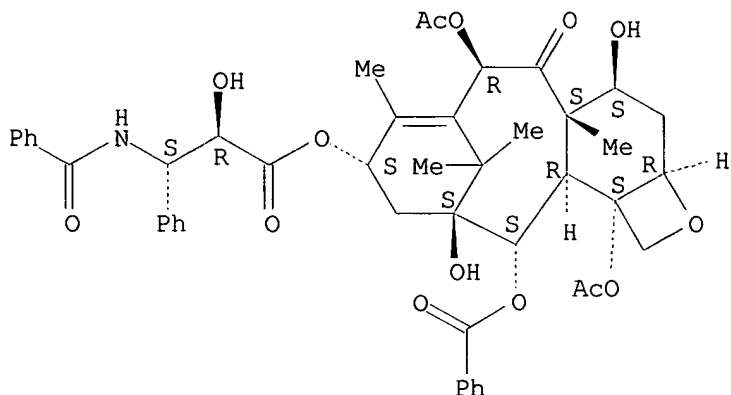
RN 23214-92-8 CAPLUS
 CN 5,12-Naphthacenedione, 10-[(3-amino-2,3,6-trideoxy-.alpha.-L-lyxo-hexopyranosyl)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(hydroxyacetyl)-1-methoxy-, (8S,10S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 33069-62-4 CAPLUS
 CN Benzenepropanoic acid, .beta.-(benzoylamino)-.alpha.-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (.alpha.R,.beta.S)- (9CI) (CA INDEX NAME)

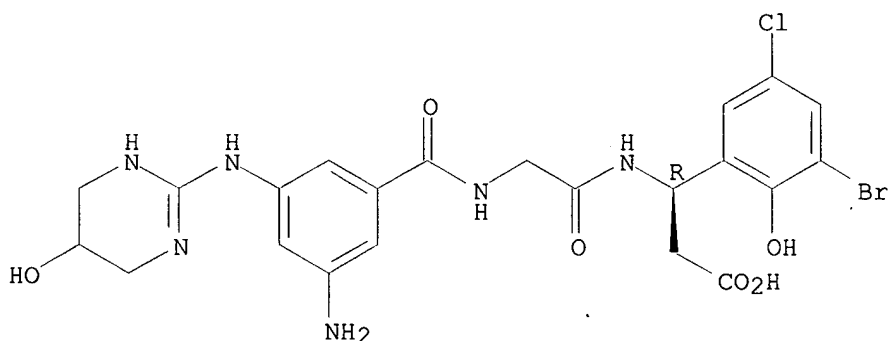
Absolute stereochemistry. Rotation (-).



RN 280105-13-7 CAPLUS

CN .beta.-Alanine, N-[3-amino-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3R)- (9CI) (CA INDEX NAME)

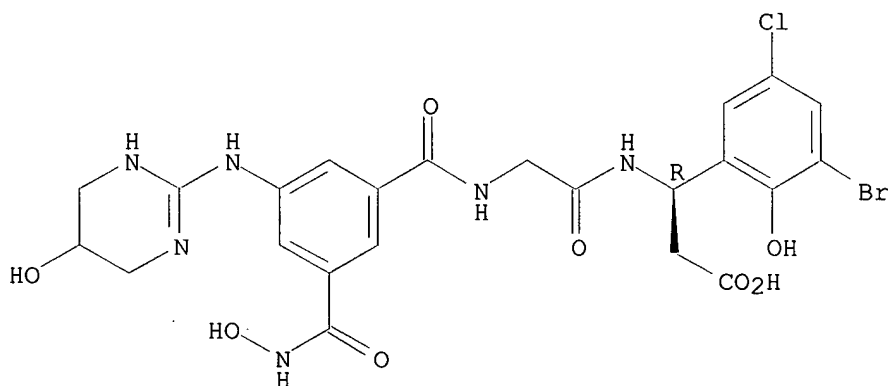
Absolute stereochemistry.



RN 280105-14-8 CAPLUS

CN .beta.-Alanine, N-[3-[(hydroxyamino)carbonyl]-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

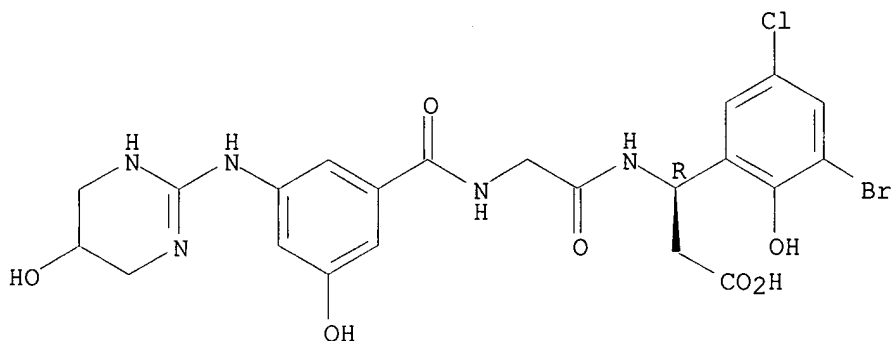


RN 280105-17-1 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-

pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-,
(3R)- (9CI) (CA INDEX NAME)

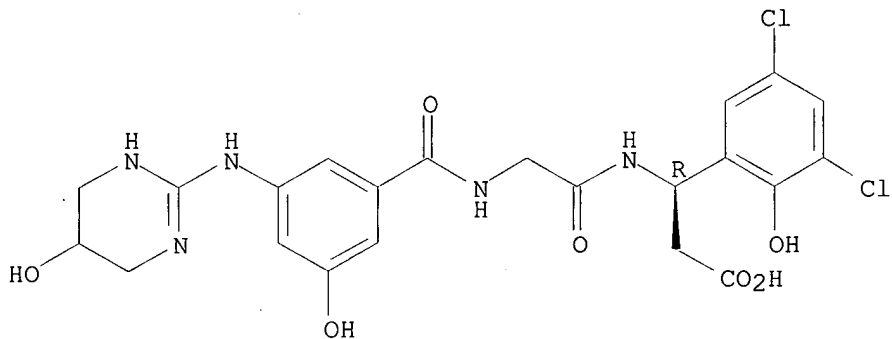
Absolute stereochemistry.



RN 280105-18-2 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, (3R)-
(9CI) (CA INDEX NAME)

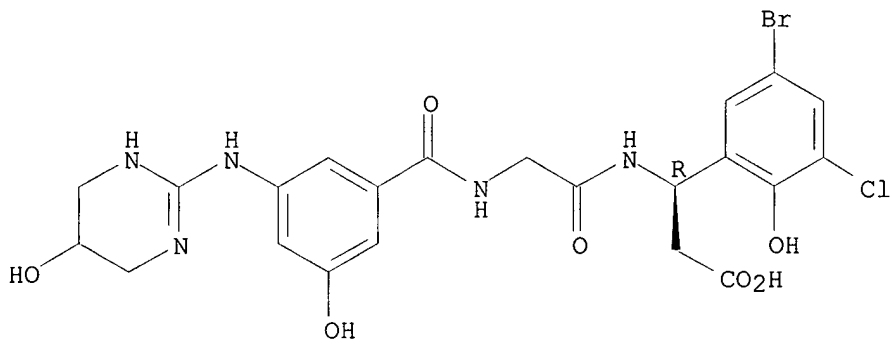
Absolute stereochemistry.



RN 280105-19-3 CAPLUS

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)-,
(3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L65 ANSWER 9 OF 10 USPATFULL

ACCESSION NUMBER: 2000:21717 USPATFULL
TITLE: Meta-guanidine, urea, thiourea or azacyclic amino
benzoic acid compounds and derivatives thereof
INVENTOR(S): Ruminski, Peter Gerrard, Ballwin, MO, United States
Clare, Michael, Skokie, IL, United States
Collins, Paul Waddell, Deerfield, IL, United States
Desai, Bipinchandra Nanubhai, Vernon Hills, IL, United States
Lindmark, Richard John, St. Louis, MO, United States
Rico, Joseph Gerace, Ballwin, MO, United States
Rogers, Thomas Edward, Ballwin, MO, United States
Russell, Mark Andrew, Gurnee, IL, United States
PATENT ASSIGNEE(S): G. D. Searle & Co., Chicago, IL, United States (U.S.
corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6028223		20000222
APPLICATION INFO.:	US 1996-713555		19960827 (8)

	NUMBER	DATE
PRIORITY INFORMATION:	US 1995-3277P	19950830 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Robinson, Allen J.	
ASSISTANT EXAMINER:	Qazi, Sabiha N.	
LEGAL REPRESENTATIVE:	Kovacevic, Cynthia S.	
NUMBER OF CLAIMS:	36	
EXEMPLARY CLAIM:	1	
LINE COUNT:	11114	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention relates to a class of compounds represented by the
Formula I ##STR1## or a pharmaceutically acceptable salt thereof,
wherein A is ##STR2## pharmaceutical compositions thereof and methods of
using such compounds and compositions as .alpha..sub.v .beta..sub.3
antagonists.

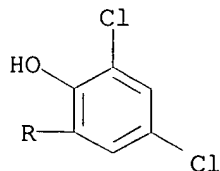
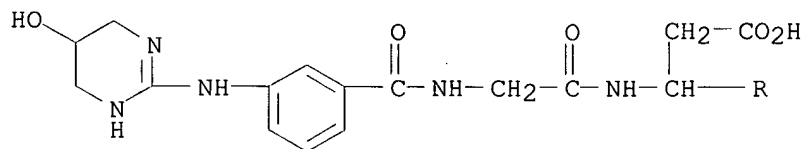
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 188811-72-5P 188811-73-6P

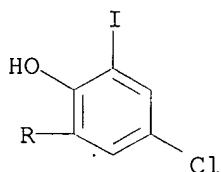
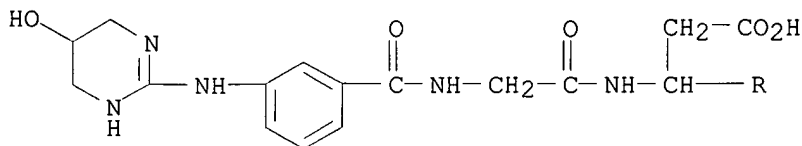
(prepn. of meta-guanidino, -ureido, -thioureido, or -azacyclic-amino
benzoic acid derivs. as integrin antagonists)

RN 188811-72-5 USPATFULL

CN .beta.-Alanine, N-[3-[(1,4,5,6-tetrahydro-5-hydroxy-2-
pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)- (9CI)
(CA INDEX NAME)



RN 188811-73-6 USPATFULL
CN .beta.-Alanine, N-[3-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-chloro-2-hydroxy-3-iodophenyl)-(9CI) (CA INDEX NAME)



L65 ANSWER 10 OF 10 USPATFULL
ACCESSION NUMBER: 2000:4813 USPATFULL
TITLE: Meta-azacyclic amino benzoic acid compounds and derivatives thereof
INVENTOR(S): Rogers, Thomas E., Ballwin, MO, United States
Ruminski, Peter G., Dardenne Prairie, MO, United States
PATENT ASSIGNEE(S): G. D. Searle & Co., Chicago, IL, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6013651		20000111
APPLICATION INFO.:	US 1998-34758		19980304 (9)
RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 1996-713555, filed on 27 Aug 1996		

	NUMBER	DATE
PRIORITY INFORMATION:	US 1995-3277P	19950830 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Dees, Jose' G.	
ASSISTANT EXAMINER:	Qazi, Sabiha N.	
LEGAL REPRESENTATIVE:	Kovacevic, Cynthia S.	
NUMBER OF CLAIMS:	36	
EXEMPLARY CLAIM:	1	
LINE COUNT:	2002	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention is directed to compounds of the formula ##STR1## and pharmaceutically acceptable salts and isomers thereof.

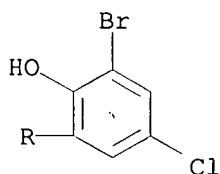
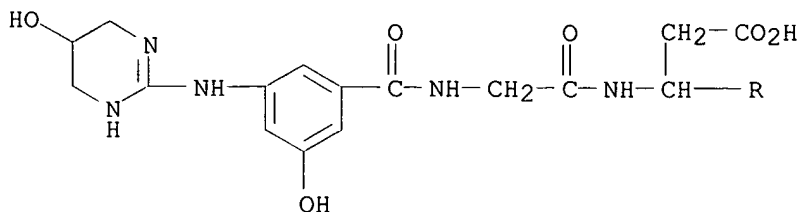
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 243135-63-9P 243135-65-1P 243135-66-2P
243135-67-3P 243135-68-4P 243135-69-5P
243135-70-8P 243135-71-9P 243135-72-0P
243135-73-1P 243135-74-2P 243135-75-3P
243135-76-4P 243135-77-5P 243135-80-0P
243135-81-1P 243135-82-2P 253866-54-5P
253866-55-6P

(prepn. of [[[(pyrimidinylamino)benzoyl]amino]acetyl]amino]benzenepropanoic acid derivs. as .alpha.v.beta.3 integrin antagonists)

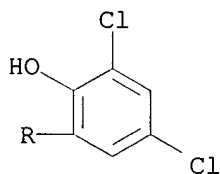
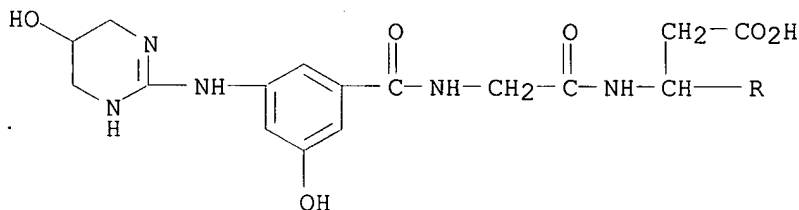
RN 243135-63-9 USPATFULL

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-(9CI) (CA INDEX NAME)



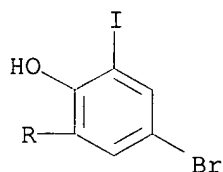
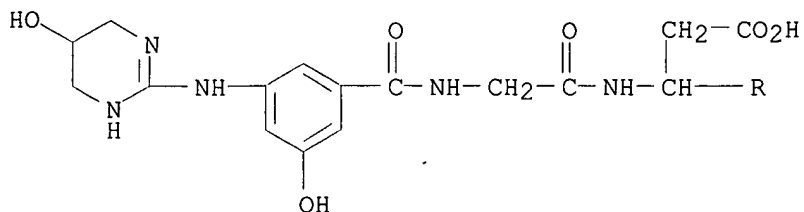
RN 243135-65-1 USPATFULL

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-(9CI) (CA INDEX NAME)



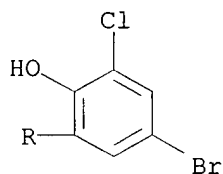
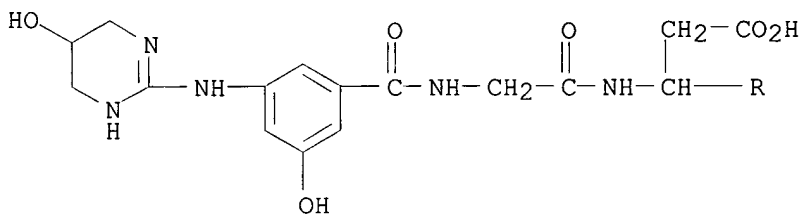
RN 243135-66-2 USPATFULL

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-iodo-2-hydroxyphenyl)-(9CI) (CA INDEX NAME)



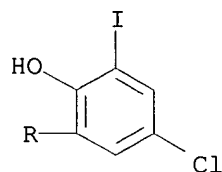
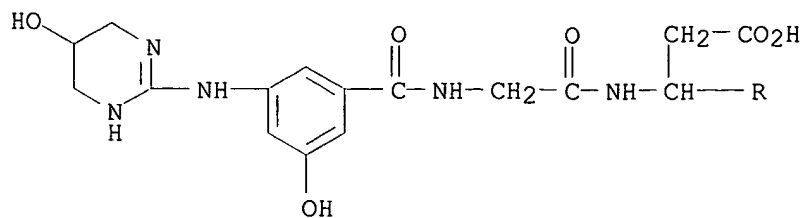
RN 243135-67-3 USPATFULL

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)-(9CI) (CA INDEX NAME)



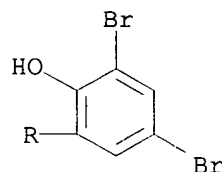
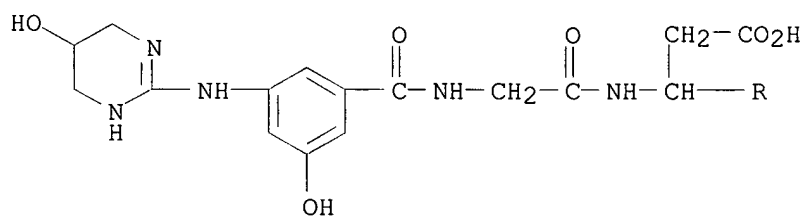
RN 243135-68-4 USPATFULL

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-chloro-3-iodo-2-hydroxyphenyl)-(9CI) (CA INDEX NAME)



RN 243135-69-5 USPATFULL

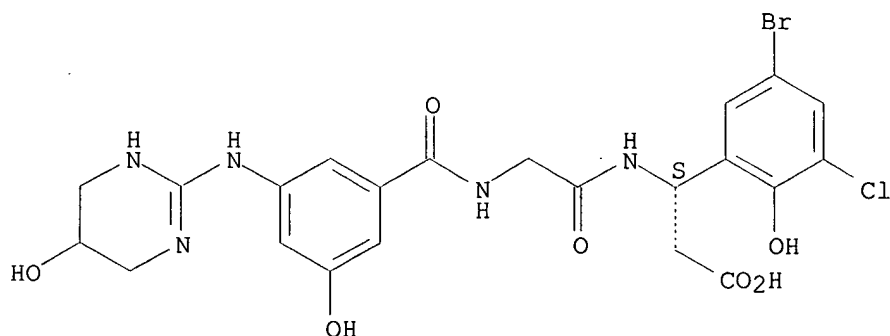
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dibromo-2-hydroxyphenyl)- (9CI)
(CA INDEX NAME)



RN 243135-70-8 USPATFULL

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-3-chloro-2-hydroxyphenyl)-, (3S)- (9CI) (CA INDEX NAME)

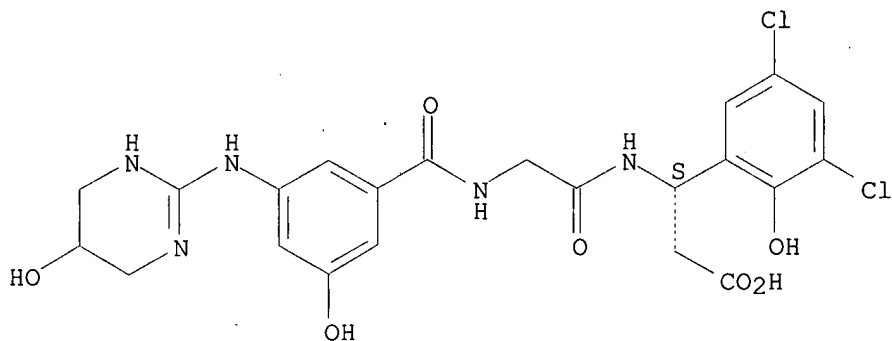
Absolute stereochemistry.



RN 243135-71-9 USPATFULL

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, monohydrochloride, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

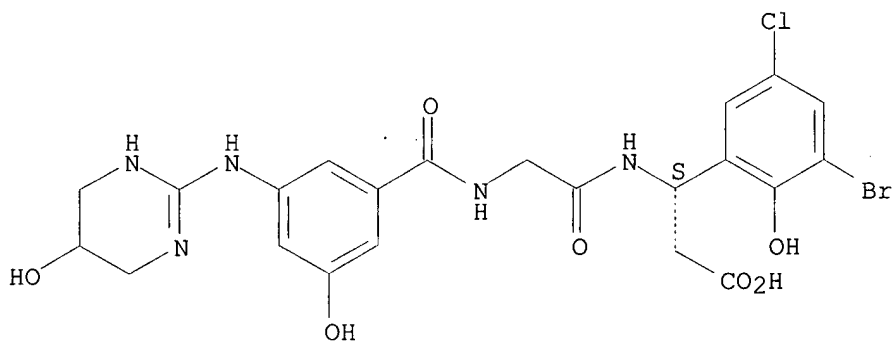


● HCl

RN 243135-72-0 USPATFULL

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 243135-73-1 USPATFULL

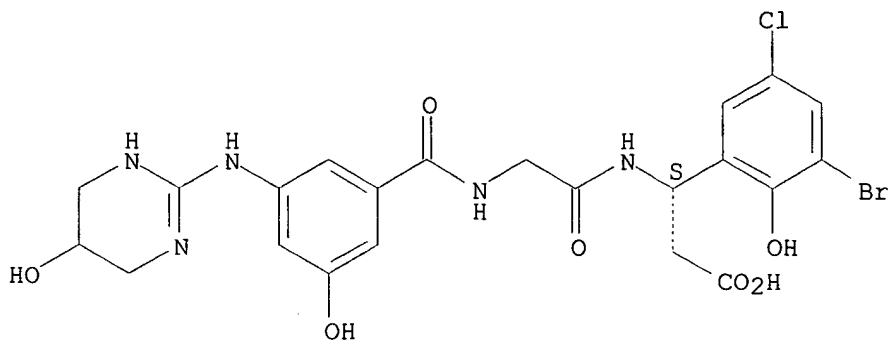
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3S)-, trifluoroacetate (10:17) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 243135-72-0

CMF C22 H23 Br Cl N5 O7

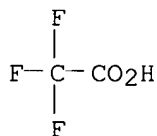
Absolute stereochemistry.



CM 2

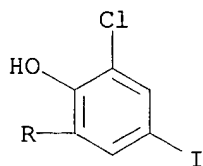
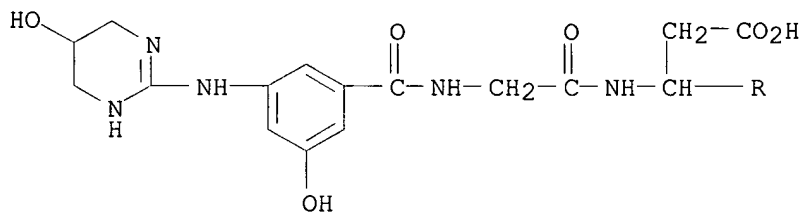
CRN 76-05-1

CMF C2 H F3 O2



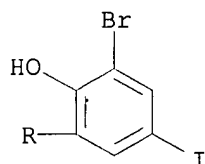
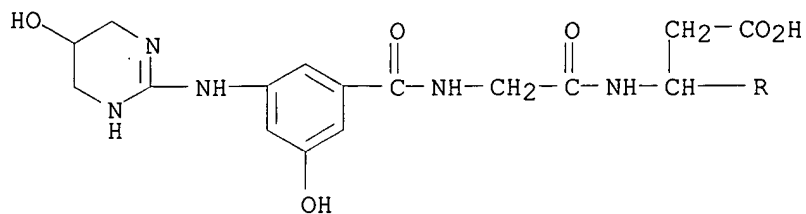
RN 243135-74-2 USPATFULL

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-chloro-5-iodo-2-hydroxyphenyl)-
(9CI) (CA INDEX NAME)



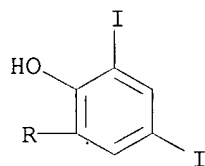
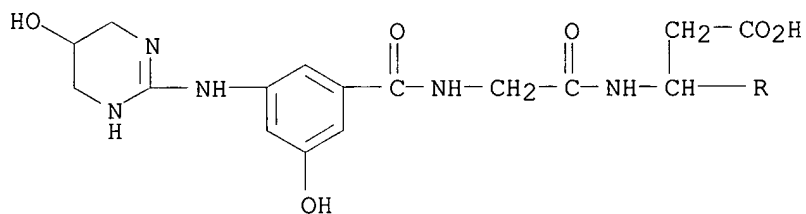
RN 243135-75-3 USPATFULL

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-iodo-2-hydroxyphenyl)-
(9CI) (CA INDEX NAME)



RN 243135-76-4 USPATFULL

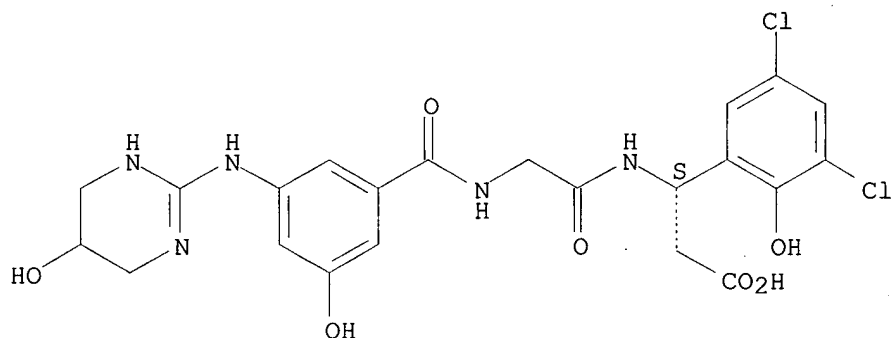
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-diiodo-2-hydroxyphenyl)- (9CI)
(CA INDEX NAME)



RN 243135-77-5 USPATFULL

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, (3S)- (9CI) (CA INDEX NAME)

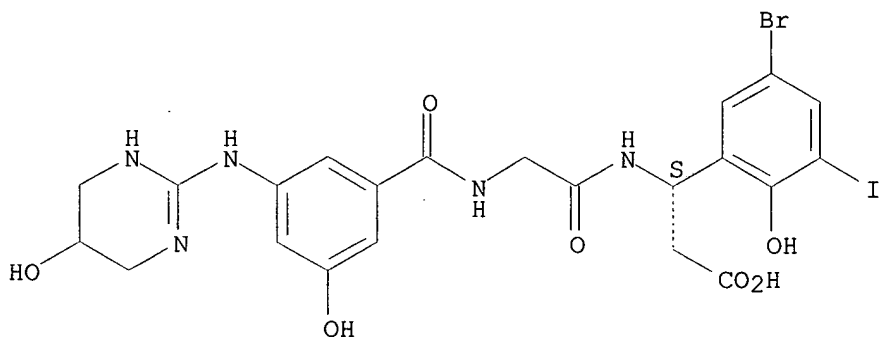
Absolute stereochemistry.



RN 243135-80-0 USPATFULL

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-2-hydroxy-3-iodophenyl)-, (3S)- (9CI) (CA INDEX NAME)

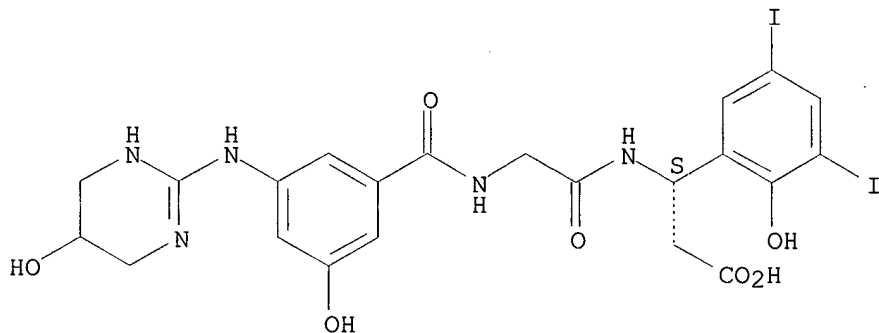
Absolute stereochemistry.



RN 243135-81-1 USPATFULL

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-diiodo-2-hydroxyphenyl)-, (3S)- (9CI) (CA INDEX NAME)

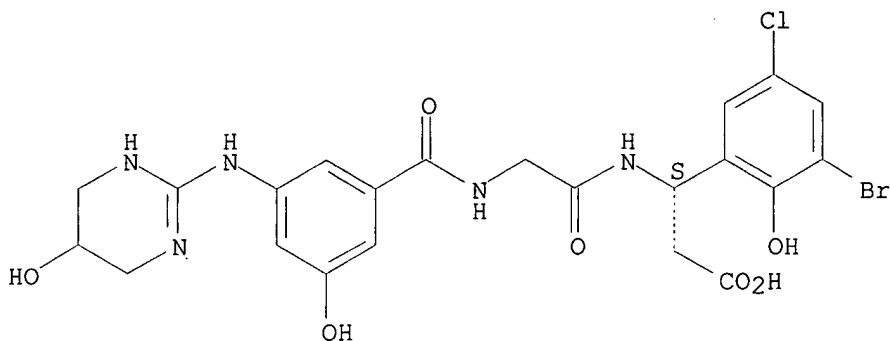
Absolute stereochemistry.



RN 243135-82-2 USPATFULL

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, monohydrochloride, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

RN 253866-54-5 USPATFULL

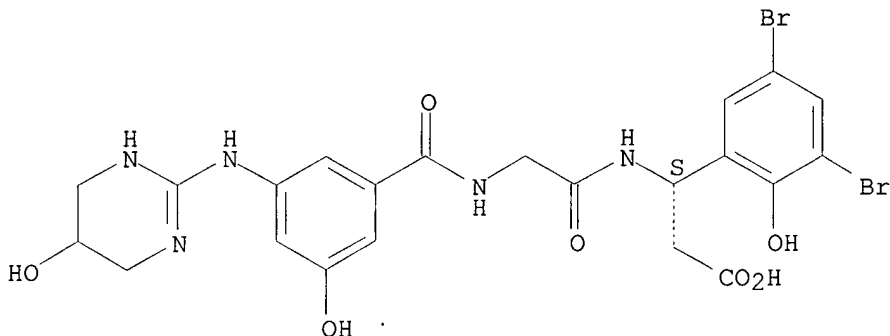
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dibromo-2-hydroxyphenyl)-, (3S)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 243135-78-6

CMF C22 H23 Br2 N5 O7

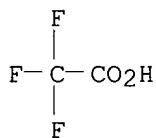
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 253866-55-6 USPATFULL

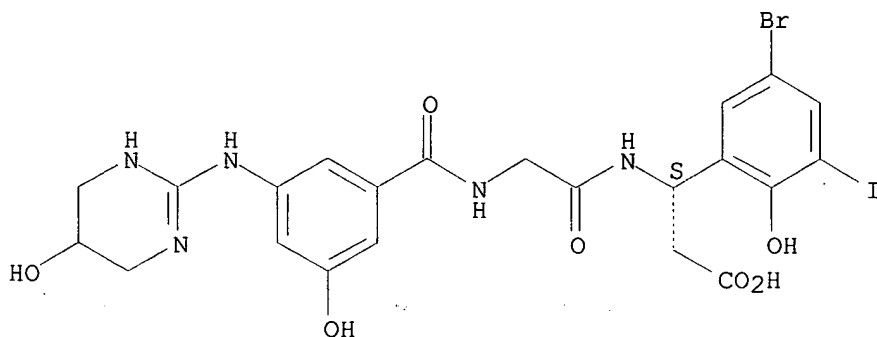
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(5-bromo-2-hydroxy-3-iodophenyl)-, (3S)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 243135-80-0

CMF C22 H23 Br I N5 O7

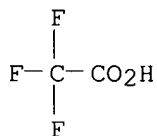
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



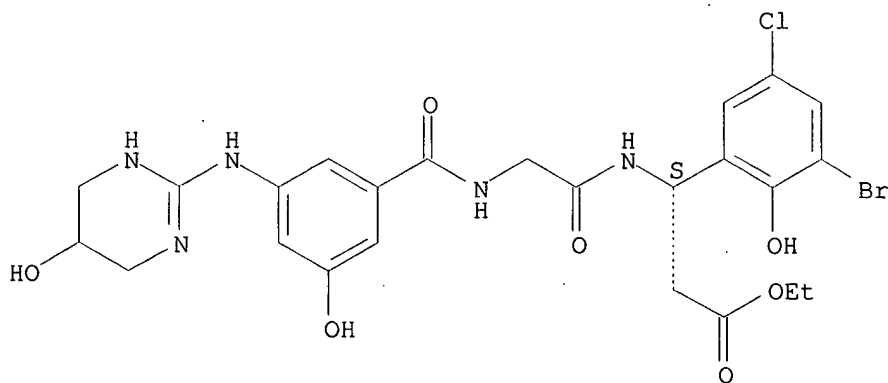
IT 243136-20-1P 253866-56-7P

(prepn. of [(((pyrimidinylamino)benzoyl]amino]acetyl]amino]benzeneprop
anoic acid derivs. as .alpha.v.beta.3 integrin antagonists)

RN 243136-20-1 USPATFULL

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-
pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-,
ethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 253866-56-7 USPATFULL

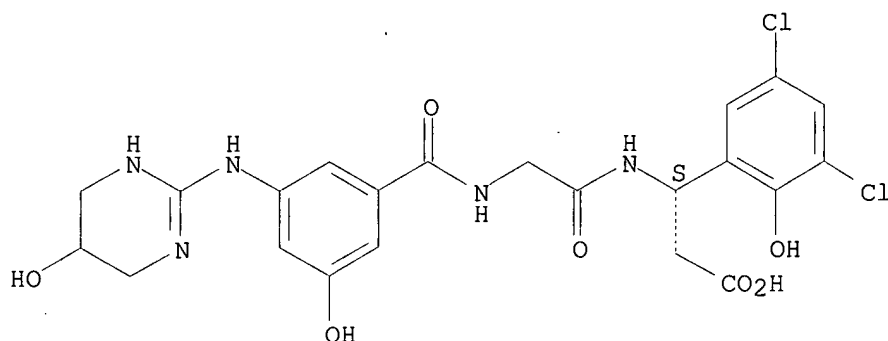
CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3,5-dichloro-2-hydroxyphenyl)-, (3S)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 243135-77-5

CMF C22 H23 Cl2 N5 O7

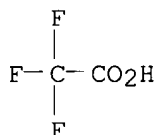
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



=> fil cancer medline drugu biosis embase

FILE 'CANCERLIT' ENTERED AT 17:19:22 ON 17 MAR 2003

FILE 'MEDLINE' ENTERED AT 17:19:22 ON 17 MAR 2003

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